

*Selected Works*  
*of*  
**HANS A  
BETHE**  
*With Commentary*

**Hans A Bethe**

***Selected Works***

**HANS A  
BETHE**

## **World Scientific Series in 20th Century Physics**

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***of***  
**HANS A**  
**BETHE**

***With Commentary***

**Hans A Bethe**

*Cornell University*



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## Preface

This book contains a selection of my publications of the 70 years during which I have been active. For each paper, I have written a historical note. Some papers, like "The Neutrino" and "The Maximum Energy Obtainable from the Cyclotron" turned out to be unduly pessimistic. The paper on Shock Waves with Teller was never published in a legitimate journal but was widely used. I hope the reader will find some of the papers interesting, as I still do.

*Hans A. Bethe*

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*Selected Works*

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BETHE**

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## **Splitting of Terms in Crystals**

*Ann. Physik* **3**, 133–206 (1929)

If an atom is placed in a crystal, its energy levels are split. The splitting depends on the symmetry of the location of the atom in the crystal. The splitting is derived here from group theory. This paper has been widely used, especially by physical chemists.

# SPLITTING OF TERMS IN CRYSTALS

Hans A. Bethe

COMPLETE ENGLISH TRANSLATION

[From: Annalen der Physik, Volume 3, pp. 133-206 (1929)]



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## SPLITTING OF TERMS IN CRYSTALS

Hans A. Bethe

(With 8 Figures)

The influence of an electric field of prescribed symmetry (crystalline field) on an atom is treated wave-mechanically. The terms of the atom split up in a way that depends on the symmetry of the field and on the angular momentum  $\ell$  (or  $j$ ) of the atom. No splitting of  $s$  terms occurs, and  $p$  terms are not split up in fields of cubic symmetry. For the case in which the individual electrons of the atom can be treated separately (interaction inside the atom turned off) the eigenfunctions of zeroth approximation are stated for every term in the crystal; from these there follows a concentration of the electron density along the symmetry axes of the crystal which is characteristic of the term. - The magnitude of the term splitting is of the order of some hundreds of  $\text{cm}^{-1}$ . - For tetragonal symmetry, a quantitative measure of the departure from cubic symmetry can be defined, which determines uniquely the most stable arrangement of electrons in the crystal.

§ 1. Introduction

There are two immediately evident points of departure for the wave mechanics of crystals: on one hand, we may treat the crystal as a single whole, and accordingly describe it in terms of a spatially periodic potential and eigenfunctions of the same spatial periodicity, whose modulation by the more detailed structure of the atoms contained in the crystal is included only in the second approximation. This method has primarily been used by Bloch<sup>1</sup> for the treatment of the electric conductivity, and seems particularly suitable in the case of electrons that are to a considerable degree "free". On the other hand, one can start with the free atom and treat its perturbation in the crystal in a way analogous to the method of London and Heitler<sup>2</sup>; one will be able to use this procedure primarily for the calculation of lattice energies, lattice spacings, etc.

There are two reasons to expect a perturbation of the free atom on its inclusion in a crystal: on one hand, the atom will enter into exchange of electrons with the other atoms of the crystal, i.e., its permutation group is changed. This exchange effect will have to be treated in a way quite analogous to the case of a molecule, there being at most a purely quantitative difference in regard to the number of neighbors with which the exchange can take place. On the other hand, there acts on the atom in the crystal an electric field arising from the other atoms

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<sup>1</sup>F. Bloch, Ztschr. f. Phys. Vol. 52, p. 555 (1929).

<sup>2</sup>F. London and W. Heitler, Ztschr. f. Phys. Vol. 44, p. 455 (1927).

which has a definite symmetry, which removes the directional degeneracy of the free atom. The qualitative difference between the molecule problem and the crystal problem is to be sought in this different spatial symmetry. In this paper, we shall deal with the specific perturbations of the free atom that are occasioned by the symmetry of the crystal, without at first going into the question of the electron-exchange phenomena for the atoms of the crystal; thus, we shall at the same time obtain a starting point for the treatment of these latter phenomena.

An electric field of definite symmetry will cause a splitting of the terms of the unperturbed atom that is analogous to the Stark-effect splitting and will just be characteristic for the symmetry of the field, i.e., for the symmetry of the situation of the atom in the crystal. The number of components into which a term of the free atom is split increases with decreasing symmetry. The amount of the splitting can be of very different orders of magnitude, and in regard to this one will have to distinguish three cases.

1. Stark-effect splitting in the crystalline field large in comparison with the separation of different multiplets: the effect of the crystalline field on the atom overcomes the interaction of the electrons in the atom and in first approximation removes the coupling between them. We then begin with a model of the free atom in which only the occupation numbers of the quantum cells specified by the principal quantum number  $n_i$  and the azimuthal quantum number  $l_i$  (of the individual electron) are prescribed, and the term splitting corresponding to the exchange degeneracy is left out of account. (The electrostatic interactions of the electrons can be included, say, by the Hartree method of the self-consistent field.)

In the first approximation we then consider the perturbation of individual electrons outside closed shells by the field of the other atoms in the crystal, i.e., the possible orientations of the orbital angular momentum  $l_i$  of the individual electron with respect to the crystal axes, and the "Stark-effect splitting" of the terms of the atom that is thus produced. In the second approximation, account would have to be taken of the electron exchange inside the atom; this in general brings about a further splitting of the terms, naturally of the order of magnitude of the separation between different multiplets of the free atom. Finally, the interaction between orbital angular momentum and spin again produces the multiplet splitting in the usual way.

2. Crystal splitting of intermediate size, i.e., small in comparison with the separation of different multiplets, but large in comparison with the differences within a single multiplet. In this (probably the most frequent) case, we must start

with the free atom including the term splitting by exchange degeneracy, but without taking into account the interaction of spin and orbit. Then this atom has to be inserted into the crystal, and we must examine the orientations of its total orbital angular momentum with respect to the axes of the crystal and the corresponding term values, and finally study the interaction between spin and orbit for fixed orientation of the latter in the crystal.

3. Crystal splitting small in comparison with the separations within a multiplet. The quite "finished" atom with account already taken of the interaction between electronic orbits and spins is subjected to perturbations by the electric field of the crystal. This means that the vector that receives an orientation relative to the crystal axes is the total angular momentum  $j$  of the atom, and no longer, as in cases 1 and 2, the orbital angular momentum, because this latter vector remains firmly coupled to the spin, whereas in cases 1 and 2 the coupling was removed by the crystalline field.

We shall use the following quantum numbers to describe the Stark-effect splitting:

$\lambda$  azimuthal crystal quantum number to specify the orientation of the orbital angular momentum of the atom in the crystal.

$\lambda_i$  azimuthal crystal quantum number of the individual ( $i$ th) electron.

$l_i$  ordinary azimuthal quantum number of the individual electron in the free atom.

$\mu$  inner crystal quantum number (orientation of the total angular momentum  $j$  of the atom in the crystal).

Since in the case of crystal quantum numbers we are in general not dealing with "true" quantum numbers, which can be interpreted as angular momentum around an axis or something of that sort, but only with distinctions between different group-theoretical representation properties of the individual terms, we write them not as numbers, but as Greek letters.

An atom is then characterized by the following quantum numbers, in the three cases mentioned above:

1. Large crystal splitting:  $n_i, l_i, \lambda_i, \lambda, \mu$ .
2. Intermediate crystal splitting:  $n_i, l_i, l, \lambda, \mu$ .
3. Small crystal splitting:  $n_i, l_i, l, j, \mu$ .

For the present, we shall treat the three possible cases - orientation of the orbital angular momentum of the individual electron, of the total orbital angular

momentum, or of the total angular momentum of the atom in the crystal - together and make group-theoretical calculations of the number of components into which a term splits for given angular momentum (representation of the rotation group) and given symmetry of the situation of the atom in the crystal. The case of the orientation of a half-integral total angular momentum (double-valued representation of the rotation group) will have to be treated separately. We shall also indicate the angle-dependent factors of the zero-order eigenfunctions belonging to the individual components resulting from the splitting, which will be required for calculations of the exchange effects. We shall then discuss separately the three cases distinguished by the order of magnitude of the crystal splitting, paying particular attention in this connection to the symmetry of the electron density distribution. Finally we shall calculate the splitting for ionic crystals.

### I. GROUP-THEORETICAL SOLUTION

#### §2. Outline of the Solution

As is well known, the Schrödinger differential equation of the free atom is invariant with respect to arbitrary rotations of the coordinate system and to an inversion in the nucleus (and with respect to exchange of the electrons, which, however, is not of interest to us for the present). Its substitution group<sup>1</sup> includes, with other factors, the rotation group of the sphere, which possesses one irreducible representation of each dimensionality  $2l + 1$  ( $l = 0, 1, 2, \dots$ ).

If we now insert the atom into a crystal, then the symmetry of the potential energy is reduced from spherical symmetry to the symmetry of the position that the atom occupies in the crystal, e.g., for insertion into a crystal of the NaCl type to cubic-holohedral symmetry, for the ZnS type to cubic-hemihedral symmetry. The substitution group of the Schrödinger differential equation for the atom in question now includes only such symmetry operations as leave the position of the nucleus of this atom unchanged and at the same time carry the entire crystal over into itself (symmetry group of the crystal atom). The way to deal with such a diminishing of the symmetry has been indicated in general by Wigner. What is required is just to accomplish the reduction of the representation of the original substitution group that belongs to a definite term of the unperturbed atom, regarding it as a representation of the new substitution group, which indeed is a subgroup of the former group; one thus obtains the number and multiplicities of the terms into which the given unperturbed term breaks up when the symmetry is diminished in the way in question. As is well known, for this, it makes no difference whether

<sup>1</sup> E. Wigner, Ztschr. f. Phys. Vol. 43, p. 624. (1927).

the perturbation is small or large, or in general what its detailed form is, nor whether one calculates the perturbation energy in first order or in arbitrarily high order: The specification of a definite symmetry of the perturbation potential is entirely sufficient.

To accomplish the reduction of the  $(2l+1)$ -dimensional representation of the rotation group, taken as a representation of a definite crystal symmetry group (for example, the octahedral group), we apply the fundamental theorem of group theory: Every reducible representation of a group can be decomposed into its irreducible constituents in one and only one way, and in the reducible representation, the character of each group element is equal to the sum of the characters that belong to the element in the irreducible representations. Accordingly we must know the character of every symmetry operation of the crystal that leaves the nucleus of the atom in its position, both in the irreducible representations of the substitution group of the crystal atom and in the irreducible representations of the substitution group of the free atom.

Every symmetry operation of the crystal atom can now be made up of a pure rotation and possibly an inversion in the nucleus, just as for the symmetry operations of the free atom. But we need only calculate the character of a prescribed rotation in the  $(2l+1)$ -dimensional representation of the rotation group; if one adjoins to the rotation an inversion, the character is simply multiplied by +1 or -1, according to whether one is dealing with a positive or a negative term<sup>1</sup>. The most general rotation is that around an arbitrary axis through the angle  $\phi$ . Its simplest representation is given by the transformation of the spherical harmonics with lower index  $l$  referred to the axis of rotation:

$$f_\mu(x) = P_l^\mu(\cos \theta) e^{i\mu\varphi}$$

Our rotation  $R$  is to leave  $\theta$  unchanged and carry  $\varphi$  over into  $\varphi + \phi$ , and thus takes  $f_\mu(x)$  over into

$$f_\mu(Rx) = P_l^\mu(\cos \theta) e^{i\mu(\varphi+\phi)}$$

i.e., our rotation is represented by the matrix<sup>1</sup>

---

<sup>1</sup>Cf. E. Wigner and J. v. Neumann, Ztschr. f. Phys. Vol. 49, p. 73, 91 (1928).

$$\begin{pmatrix} e^{-i\frac{\pi}{3}\phi} & 0 & \dots & \dots & 0 \\ 0 & e^{-i(\frac{\pi}{3}-2)\phi} & \dots & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & \dots & e^{i\frac{\pi}{3}\phi} \end{pmatrix}$$

with the character

$$\chi(\phi) = \frac{\sin(i + \frac{1}{3})\phi}{\sin \frac{1}{3}\phi} \quad (1)$$

### § 3. Holohedral and Hemihedral Symmetry

If an atom in the crystal possesses holohedral symmetry, it must be a symmetry center of the whole crystal. Then its symmetry operations can be classified into two categories of equal numbers of elements, the pure rotations on one hand and the rotations with reflection on the other. The pure rotations form an invariant subgroup of the group. From every class of pure rotations, a class of reflections or rotations with reflection arises by multiplication with the inversion in the nucleus.

For, let us assume that  $C$  is a class of the invariant subgroup  $N$  consisting of the pure rotations, i.e., if  $X$  is any element of the invariant subgroup:

$$X^{-1} C X = C$$

Let  $J$  be the inversion, which naturally commutes with every rotation ( $J^2 = E$ ). It then follows that  $C$  is also a class in the entire group:

$$(J X)^{-1} C J X = C$$

Furthermore,  $JC$  also forms a class of the group:

$$X^{-1} J C X = J C$$

q. e. d. (Cf. example in the following section).

Accordingly, the group consists of precisely twice as many elements in precisely twice as many classes as the invariant subgroup in question, and therefore possesses twice as many representations as the latter, namely, first the positive representations, in which the inversion is represented by the unit matrix and the inversion class  $JC$  has the same character as the rotation class  $C$ , and second the negative representations, in which the inversion is represented by the negative unit matrix and multiplication of a class  $C$  by the inversion results in multiplying the character by -1. By comparison with the definition of Wigner and von Neumann<sup>1</sup>

<sup>1</sup>E Wigner and J. v. Neumann, loc. cit. p. 91.

one sees at once that: In a position of holohedral symmetry, a positive term of the free atom breaks up into nothing but positive crystal terms, a negative term of the free atom into nothing but negative. Beyond this one need bother no further with the inversion, but has only to carry out the reduction of the spherical rotation group taken as representations of the group consisting of the pure rotations of the crystal around the nucleus of the atom, which we shall call the crystal rotation group (tetragonal, hexagonal rotation group).

By omission of half of all the symmetry elements and half of all symmetry classes, there arises from the holohedral group a hemihedral symmetry group, provided that the remaining elements form a group. If the inversion also belongs to the elements of the hemihedral symmetry group, then one can use the same argument as for holohedral symmetry and confine the consideration to the elements of the group consisting of pure rotations. The splitting up of a term of the free atom then in general gives more components than for holohedral symmetry. If the inversion is not an element of the hemihedral symmetry group, then by multiplication by the inversion one can complete the hemihedral group to the holohedral symmetry group, where as above two classes of the holohedral group correspond to each class of the hemihedral group. Accordingly every hemihedral symmetry group that does not contain the inversion corresponds class for class with the invariant subgroup of the holohedral group that consists of the pure rotations, and thus also has precisely the same representations as the latter. (The invariant subgroup itself of course also forms a hemihedral symmetry group, which we can designate as rotational hemihedrism, but besides this other hemihedrisms without an inversion center are also conceivable.)

We shall now call a representation of a hemihedral symmetry group positive-equal to a representation of the rotation-hemihedral group if corresponding classes of the two groups have the same character throughout. We will call two representations of the groups negative-equal if only the rotation classes of the hemihedral symmetry group have exactly the same character as the corresponding classes of the rotation-hemihedral group, and on the other hand the characters of the reflection classes of the hemihedral symmetry group are equal to the negatives of those of the corresponding rotation classes in the representation of the rotation-hemihedral group used for the comparison.

For a hemihedral symmetry of the position of the atom in the crystal in which it is not an inversion center, a term of the free atom splits up into exactly as many components as for the associated holohedral symmetry. The representations

of the terms that arise from a positive term of the free atom in a position of hemihedral symmetry are positive-equal to the irreducible representations of the crystal rotation group (rotational hemihedrism) which one obtains on the reduction of that representation of the spherical rotation group that belongs to the term of the free atom. On the other hand, from a negative term of the free atom there arise, for a position of hemihedral symmetry, terms whose representations are negative-equal to the corresponding representations of the crystal rotation group.

We now proceed to the consideration of particular symmetry groups.

#### § 4. Cubic-Holohedral Symmetry (e.g., NaCl, Ca in CaF<sub>3</sub>)

We assume that all the rotation axes and mirroring planes of the cubic-holohedral symmetry can be chosen to pass through the nucleus of the atom under consideration. The 24 pure rotations of the cubic-holohedral symmetry group, which are identical with the rotations of the octahedral group, fall into five classes:

E identity.

C<sub>3</sub> rotations around the three 4-fold axes (cube edges) through angle  $\pi$  (3 elements).

C<sub>3</sub> rotations around the 4-fold axes by  $\pm \pi/2$  (6 elements).

C<sub>4</sub> rotations around the six 2-fold axes (face diagonals of the cube) by  $\pi$  (6 elements).

C<sub>5</sub> rotations around the four 3-fold axes (body diagonals of cube) by  $\pm 2\pi/3$  (8 elements).

By multiplication with the inversion there arise from these:

J inversion.

JC<sub>3</sub> reflections in the planes perpendicular to the 4-fold axes (3 elements).

JC<sub>3</sub> rotation-reflections around the 4-fold axes (rotation by  $\pm\pi/2$  + reflection in the plane perpendicular to the axis) (6 elements).

JC<sub>4</sub> reflections in the planes passing through a 4-fold axis and a 2-fold axis perpendicular to it (6 elements).

JC<sub>5</sub> rotation-reflections around the 3-fold axes (6-fold rotation-reflection axes); (rotation by  $\pm\pi/3$  and reflection in the plane perpendicular to the axis) (8 elements).

The octahedral group consisting of 24 elements accordingly possesses five irreducible representations. The sum of the squares of the dimensionalities of all the representations must be equal to the number of elements in the group; accordingly,

we must write 24 as the sum of 5 squares. The only possibility is the decomposition

$$24 = 9^2 + 8^2 + 2^2 + 1^2 + 1^2$$

That is, the octahedral group possesses two three-dimensional, one two-dimensional, and two one-dimensional representations. Every term of the unperturbed atom of higher than three-fold directional degeneracy must therefore split up in a crystal of cubic-holohedral symmetry. In order now to calculate the characters of the representations of the octahedral group, we start with the formula<sup>1</sup>

$$h_i h_k \chi_i \chi_k = \chi_1 \sum c_{ikl} h_l \chi_l$$

The products of classes by twos give:

$$\begin{aligned} C_3^2 &= 8E + 2C_2 & C_2 C_3 &= C_3 + 2C_4 \\ C_2^2 &= 6E + 2C_3 + 3C_5 & C_2 C_4 &= 2C_3 + C_4 \\ C_4^2 &= 6E + 2C_2 + 3C_6 & C_2 C_6 &= 3C_6 \\ C_5^2 &= 8E + 8C_2 + 4C_6 & C_3 C_4 &= 4C_3 + 3C_5 \\ && C_3 C_5 &= C_4 C_5 = 4C_3 + 4C_4 \end{aligned}$$

From this we get the following systems of characters:

TABLE 1

Representation	Class				
	E	C <sub>2</sub>	C <sub>3</sub>	C <sub>4</sub>	C <sub>6</sub>
$\Gamma_1$	1	1	1	1	1
$\Gamma_2$	1	1	-1	-1	1
$\Gamma_3$	2	2	0	0	-1
$\Gamma_4$	3	-1	1	-1	0
$\Gamma_5$	3	-1	-1	1	0

According to the formulas at the end of Sect. 2, in the  $(2l+1)$ -dimensional representation of the rotation group, the characters corresponding to the classes of the octahedral group are as follows:

<sup>1</sup>A. Speiser, Theorie der Gruppen, 1 Aufl. p. 163, 2 Aufl. p. 171.

$$\begin{aligned}
 \text{Class E} & \quad \text{Rotation by } \Phi = 0 \quad \chi_E = 2l + 1 \\
 \text{Classes } C_2 \text{ and } C_4 & \quad " \quad \Phi = \pi \quad \chi_2 = \chi_4 = \frac{\sin\left(l + \frac{1}{2}\right)\pi}{\sin\frac{\pi}{2}} = (-)^l \\
 \text{Class } C_3 & \quad " \quad \Phi = \frac{\pi}{2} \quad \chi_3 = \frac{\sin\left(\frac{l}{2} + \frac{1}{4}\right)\pi}{\sin\frac{\pi}{4}} = (-)^{\left[\frac{l}{2}\right]} \\
 \text{Class } C_6 & \quad " \quad \Phi = \frac{2\pi}{3} \quad \chi_6 = \frac{\sin\left(\frac{2l}{3} + \frac{1}{3}\right)\pi}{\sin\frac{\pi}{3}} \\
 & \qquad \qquad \qquad = \begin{cases} 1, & \text{for } l = 3m \\ 0, & \text{, , } l = 3m+1 \\ -1, & \text{, , } l = 3m+2 \end{cases}
 \end{aligned}$$

In detail, one has corresponding to the representations of the spherical rotation group the characters for the individual classes of the octahedral group as shown in the following table, and from them one obtains the decompositions into irreducible representations of the octahedral group shown at the right:

TABLE 2

Characters of the classes of the octahedral group in the $(2l+1)$ -dimensional representation of the rotation group						Decomposition of the $(2l+1)$ -dimensional representation of the rotation group into irreducible representations of the octahedral group	Number of Terms
$l$	$E$	$C_2$	$C_3$	$C_4$	$C_6$		
0	1	1	1	1	1	$\Gamma_1$	1
1	3	-1	1	-1	0	$\Gamma_4$	1
2	5	1	-1	1	-1	$\Gamma_1 + \Gamma_2$	2
3	7	-1	-1	-1	1	$\Gamma_3 + \Gamma_4 + \Gamma_5$	3
4	9	1	1	1	0	$\Gamma_1 + \Gamma_3 + \Gamma_4 + \Gamma_6$	4
5	11	-1	1	-1	-1	$\Gamma_3 + 2\Gamma_4 + \Gamma_5$	4
6	13	1	-1	1	1	$\Gamma_1 + \Gamma_3 + \Gamma_4 + \Gamma_6 + 2\Gamma_7$	6
12	25	1	-1	1	1	$2\Gamma_1 + \Gamma_3 + 2\Gamma_4 + 3\Gamma_6 + 3\Gamma_7$	11

According to this, S and P terms of the unperturbed atom do not split up when one places the atom in a position of cubic-holohedral symmetry in a crystal. From the D terms on, every term splits up, and into at most as many components as the value of the azimuthal quantum number  $l$ , accordingly into fewer components than appear in the Stark effect in a homogeneous field<sup>1</sup>. For  $l = 12$  (in general for  $l = 12m$ ) the characters of all classes of the octahedral group are equal to +1, only

<sup>1</sup>When two terms with the same representation appear in the reduction of the representation, these are of course nevertheless different, just as also their eigenfunctions have different detailed angular dependences and transform in the same way only for the special symmetry operations of the crystal atom. Concerning this, see Sections 11, 18, 22.

the character of the unit element being equal to 25 (or  $24m + 1$ ). Accordingly, the 25-dimensional representation of the rotation group, reduced to irreducible parts as a representation of the octahedral group, contains the regular representation exactly once, and in addition one extra occurrence of the identical representation. (Indeed, in the regular representation, all the characters are zero, except that the one of the unit element is equal to the number of elements in the group, here 24.) In general it follows that the  $[2(12m + k) + 1]$ -dimensional representation of the rotation group contains the regular representation of the octahedral group  $m$  times, and in addition, the same representations as the  $(2k + 1)$ -dimensional representation of the rotation group. If one carries out the reduction of the  $[24m - (2k + 1)]$ -dimensional representation, just the components of the  $(2k + 1)$ -dimensional representation are lacking to make up the regular representation  $m$  times.

Note: Almost the same problem as is treated in this section and in Sections 12 and 13 has been solved already by Ehlert<sup>1</sup> from a quite different approach. For him it was a matter of finding the nuclear vibration functions of prescribed Hund symmetry character with respect to interchange of the protons in a molecule of the type CH<sub>4</sub>. In this connection one is led to the investigation of the transformation of spherical surface harmonics on interchange of the vertices of a tetrahedron. These interchanges form a cubic-hemihedral group, which includes the classes E, C<sub>2</sub>, C<sub>3</sub>, JC<sub>3</sub> and JC<sub>4</sub> of the holohedral group. If, with Ehlert, one omits the interchanges that correspond to a mirroring, then there are three possible symmetry characters {1234}, {123}4, and {12}{34} for an eigenfunction, which correspond to the representations Γ<sub>1</sub> and Γ<sub>2</sub> or Γ<sub>4</sub> and Γ<sub>5</sub> or Γ<sub>3</sub> respectively, of the octahedral group. For example, one finds the number of spherical harmonics of the  $l$ th order of symmetry character {1234} if one adds the numbers of terms with the representation properties Γ<sub>1</sub> and Γ<sub>2</sub> (with respect to rotations of the octahedron) which arise for cubic symmetry from one term of the unperturbed atom with the azimuthal quantum number  $l$ . Similarly, the number of functions with the character {12}{34} is equal to twice the number of terms Γ<sub>3</sub>, because two eigenfunctions belong to each such term, and the number of functions with the symmetry character {123}4 is equal to three times the total number of terms with the representations Γ<sub>4</sub> and Γ<sub>5</sub>. In this way one obtains at once the numbers of eigenfunctions with prescribed symmetry characters as given by Ehlert. In the actual construction of the eigenfunctions, Ehlert's method is indeed probably preferable (cf. § 12, 13).

## § 5. Hexagonal, Tetragonal, and Rhombic (Holohedral) Symmetries

a) The hexagonal symmetry group contains 12 pure rotations, which fall into 6 classes:

E identity.

C<sub>2</sub> rotation by  $\pi$  around the hexagonal axis (1 element).

C<sub>3</sub> rotation by  $\pm 2\pi/3$  around the hexagonal axis (2 elements).

C<sub>4</sub> rotation by  $\pm \pi/3$  around the hexagonal axis (2 elements).

C<sub>5</sub> rotation by  $\pi$  around one of the three 2-fold axes (3 elements).

C<sub>6</sub> rotation by  $\pi$  around one of the three 2-fold axes perpendicular to those above (3 elements).

<sup>1</sup>W. Ehlert, Ztschr. f. Phys. 51, p. 8. 1928.

In addition to these, one would have the 6 reflection or rotation-reflection classes obtained by multiplying by the inversion; we do not, however, need to bother with these (§ 3). The dimensionalities of the 6 representations are found by writing 12 as a sum of 6 squares, which is possible only in the form

$$12 = 2^2 + 2^2 + 1^2 + 1^2 + 1^2 + 1^2$$

There are four one-dimensional and two two-dimensional representations of the hexagonal rotation group; accordingly, even the P terms of a free atom must split up when the atom is inserted into a crystal in a position of hexagonal-holohedral symmetry.

The products of the classes by twos give:

$$\begin{array}{ll} C_2^2 = E & C_2 C_3 = C_4 \\ C_3^2 = C_4^2 = 2E + C_3 & C_2 C_4 = C_3 \\ C_5^2 = C_6^2 = 8E + 8C_3 & C_2 C_5 = C_6 \\ C_3 C_4 = 2C_2 + C_4 & C_2 C_6 = C_3 \\ C_5 C_6 = 8C_2 + 8C_4 & C_3 C_6 = C_4 C_6 = 2C_5 \\ C_3 C_5 = C_4 C_5 = 2C_6 \end{array}$$

From this one finds for the characters of the irreducible representations of the hexagonal-holohedral group:

TABLE 3

	$E$	$C_2$	$C_3$	$C_4$	$C_5$	$C_6$
$\Gamma_1$	1	1	1	1	1	1
$\Gamma_2$	1	1	1	1	-1	-1
$\Gamma_3$	1	-1	1	-1	1	-1
$\Gamma_4$	1	-1	1	-1	-1	1
$\Gamma_5$	2	2	-1	-1	0	0
$\Gamma_6$	2	-2	-1	1	0	0

In the  $(2l+1)$ -dimensional representation of the spherical rotation group, the classes of the hexagonal rotation group have the following characters (end of § 2):

$$\chi_E = 2l+1$$

$$\chi_2 = \chi_3 = \chi_4 = (-)^l$$

$$\chi_3 = \frac{\sin \frac{2l+1}{3}\pi}{\sin \frac{\pi}{3}} = \begin{cases} 1, & \text{for } l = 3m \\ 0, & 3m + 1 \\ -1, & 3m + 2 \end{cases}$$

$$\chi_4 = \frac{\sin \frac{2l+1}{6}\pi}{\sin \frac{\pi}{6}} = \begin{cases} 1, & \text{for } l \equiv 0 \text{ or } 2 \pmod{6} \\ 2, & " l \equiv 1 \pmod{6} \\ -1, & l \equiv 3 \text{ or } 5 \pmod{6} \\ -2, & " l \equiv 4 \pmod{6} \end{cases}$$

In detail, one finds

TABLE 4

Characters of the classes of the hexagonal group in the $(2l+1)$ -dimensional representation of the spherical rotation group							Decomposition of the $(2l+1)$ -dimensional representation of the rotation group into irreducible representations of the hexagonal rotation group	Number of Terms
$l$	$E$	$C_2$	$C_3$	$C_4$	$C_5$	$C_6$		
0	1	1	1	1	1	1	$\Gamma_1$	1
1	3	-1	0	2	-1	-1	$\Gamma_2 + \Gamma_6$	2
2	5	1	-1	1	1	1	$\Gamma_1 + \Gamma_5 + \Gamma_6$	3
3	7	-1	1	-1	-1	-1	$\Gamma_2 + \Gamma_3 + \Gamma_4 + \Gamma_5 + \Gamma_6$	5
4	9	1	0	-2	1	1	$\Gamma_1 + \Gamma_3 + \Gamma_4 + 2\Gamma_5 + \Gamma_6$	6
5	11	-1	-1	-1	-1	-1	$\Gamma_1 + \Gamma_3 + \Gamma_4 + 2\Gamma_5 + 2\Gamma_6$	7
6	13	1	1	1	1	1	$2\Gamma_1 + \Gamma_3 + \Gamma_5 + \Gamma_4 + 2\Gamma_6 + 2\Gamma_6$	9

The  $[2(6m+k)+1]$ -dimensional representation of the rotation group contains the regular representation of the hexagonal group  $m$  times, and in addition the same representations of the hexagonal group as are contained in the  $(2k+2)$ -dimensional representation of the spherical rotation group. The  $(2l+1)$ -fold degenerate term of the free atom splits up, as one can easily calculate, in the hexagonal crystal into  $\left[\frac{4}{3}l\right] + 1$  terms, of which  $2\left[\frac{l}{3}\right] + 1$  are single and the other  $\left[\frac{2l-1}{3}\right] + 1$  are two-fold degenerate.

b) The tetragonal symmetry group contains 8 rotations in 5 classes:

$E$ : identity,

$C_2$ : rotation by  $\pi$  around the tetragonal axis.

$C_3$ : rotation by  $\pm\pi/2$  around the tetragonal axis (2 elements).

$C_4$ : rotation by  $\pi$  around a two-fold axis perpendicular to the tetragonal axis (2 elements).

$C_5$ : rotation by  $\pi$  around the bisectors of the angles between the above axes (2 elements).

The group possesses four one-dimensional representations and one with two dimensions; the characters are:

TABLE 5  
Character of the Tetragonal Rotation Group

	$E$	$C_2$	$C_2^l$	$C_4$	$C_4^l$
$\Gamma_1$	1	1	1	1	1
$\Gamma_2$	1	1	1	-1	-1
$\Gamma_3$	1	1	-1	1	-1
$\Gamma_4$	1	1	-1	-1	1
$\Gamma_5$	2	-2	0	0	0

The characters of the tetragonal rotations in the  $(2l+1)$ -dimensional representation of the spherical rotation group are (§ 2):

$$\begin{aligned}\chi_E &= 2l+1 \\ \chi_2 &= \chi_4 = \chi_3 = (-)^l \\ \chi_3 &= (-)^{\left[\frac{l}{2}\right]}\end{aligned}$$

From this, one obtains the decomposition of the  $(2l+1)$ -dimensional representation of the spherical rotation group into irreducible representations of the tetragonal rotation group, which can be generally stated as follows:

TABLE 6

When $l =$	$4\lambda$	$4\lambda+1$	$4\lambda+2$	$4\lambda+3$
the numbers of times $n_i$ that the representation $\Gamma_i$ occurs are:				
$\Gamma_1$	$\lambda+1$	$\lambda$	$\lambda+1$	$\lambda$
$\Gamma_2$	$\lambda$	$\lambda+1$	$\lambda$	$\lambda+1$
$\Gamma_3$	$\lambda$	$\lambda$	$\lambda+1$	$\lambda+1$
$\Gamma_4$	$\lambda$	$\lambda$	$\lambda+1$	$\lambda+1$
$\Gamma_5$	$2\lambda$	$2\lambda+1$	$2\lambda+1$	$2\lambda+2$

One can easily convince oneself that the relations between the characters are satisfied by the values given. In general the  $(2l+1)$ -fold degenerate term of the free atom splits up into  $\left[\frac{3}{2} l\right] + 1$  terms, of which  $\left[\frac{l+1}{2}\right]$  are two-fold degenerate and  $2\left[\frac{l}{2}\right] + 1$  are single.

c) Rhombic Symmetry. Each of the 4 rotations (identity and rotation by  $\pi$  around each of the three axes) forms a class by itself. The group possesses four

one-dimensional representations, and every term of the free atom splits up completely into  $2l + 1$  single terms. The same thing occurs for still lower symmetry.

### § 6. Orientation of a Half-Integral Angular Momentum in the Crystal. Double-Valued Group Representations

If the Stark effect splitting in the crystal is small in comparison with the separation of the terms of the same multiplet of the free atom, the total angular momentum  $j$  of the atom takes up an orientation in the crystal (every component of a multiplet splits up separately) (§ 1, Case 3). If now the atom to be inserted into the crystal possesses even term multiplicities (odd atomic number), the angular momentum  $j$  is half-integral, the same as for a single electron, and has a double-valued representation of the space rotation group. Thus, the rotation around an arbitrary axis by the angle  $\Phi$  has the character

$$\chi(\Phi) = \frac{\sin(j + \frac{1}{2})\Phi}{\sin \frac{1}{2}\Phi} \quad (2)$$

quite in analogy with Eq. (1). But  $j + \frac{1}{2}$  is integral, so that

$$\sin(j + \frac{1}{2})(\Phi + 2\pi) = \sin(j + \frac{1}{2})\Phi$$

whereas previously we had, for integral  $l$ ,

$$\sin(l + \frac{1}{2})(\Phi + 2\pi) = -\sin(l + \frac{1}{2})\Phi$$

Since, however, in the denominator we have

$$\sin \frac{1}{2}(\Phi + 2\pi) = -\sin \frac{1}{2}\Phi$$

it follows that for half-integral  $j$

$$\chi(2\pi, \pm)\Phi = -\chi(\Phi)$$

Every character changes its sign when a rotation through  $2\pi$  is added, i.e., every character is double-valued. Also the character of the identical rotation can be either

$$\chi(0) = 2l + 1$$

or

$$\chi(2\pi) = -(2l + 1)$$

The only character with a unique value is that for a rotation by  $\pi$  around an arbitrary axis,

$$\chi(\pi) = \chi(8\pi) = 0$$

and in general one has

$$\chi(\Phi) = \chi(4\pi - \Phi)$$

Such a double-valued representation of the spherical rotation group can of course contain only double-valued representations of the crystal rotation groups as irreducible components. In order to obtain these double-valued representations, we introduce the fiction that the crystal is not to go over into itself on rotation by  $2\pi$  around an arbitrary axis, but only on rotation by  $4\pi$ . We accordingly define a new group element R, the rotation by  $2\pi$  (around any axis whatever), and supplement the elements of the crystal rotation group by those that arise from them by multiplication by R. We shall designate the group so obtained, which has twice as many elements as the original group, as the crystal double group, and shall inquire about its irreducible representations. This accomplishes our purpose of representing every element of the simple group by two matrices (a two-valued matrix). This procedure corresponds somewhat to the construction of the Riemann surface for the study of multiple-valued functions.

The double group contains more classes than the simple group, but not twice as many. In general, the rotation by  $\Phi$  around a definite axis does not belong for the double group to the same class as the rotation around the same axis by  $2\pi \pm \Phi$ ; for the characters of the two rotations are indeed different in the reducible representations of the double group<sup>1</sup>. An exception to this is the case  $2\pi - \Phi = \Phi = \pi$ ,  $\chi(\Phi) = 0$ . All classes of rotations of the simple crystal group that contain rotations by  $\pi$  accordingly correspond to one class each of the double group, all others to two classes each. We shall find this confirmed in the study of the individual "double groups".

#### § 7. The Tetragonal Double Group

The simple group of the tetragonal rotations can be completely constructed from the two elements

A = rotation by  $\pi/2$  around the tetragonal axis,

B = rotation by  $\pi$  around any two-fold axis;

with  $A^4 = B^2 = E$  for the simple group. The classes of the simple group and the elements they contain are:

<sup>1</sup>The double-valued representations of the rotation group are indeed reducible representations of the crystal double group.

$E$  contains the element  $E = A^4$

$C_2$  contains the element  $A^2$

$C_3$  contains the elements  $A, A^3$

$C_4$  contains the elements  $B, A^2B$

$C_5$  contains the elements  $AB, A^3B$

In this group,  $(AB)^2 = E$ .

We expect that in the double group there will be two classes corresponding to each of the classes  $E$  and  $C_3$ , of the simple group, and one class corresponding to each of the others. We obtain the double group by setting

$$A^4 = B^2 = R, \quad R^2 = E$$

$R$  commutes with all other elements of the group. One obtains the following classes of the double group:

$$\begin{aligned} &E \\ &R \\ &C_3 = A^2, A^4 \\ &C_3' = A, A^3 \\ &C_3'' = A^3, A^5 \\ &C_4 = B, A^2B, A^4B = RB = B^2, A^6B = (A^2B)^3 \\ &C_5 = AB, A^3B, A^5B, A^7B \end{aligned}$$

The 16 elements of the double group accordingly fall into 7 classes, so that to determine the dimensionalities of the irreducible representations we must split 16 up into a sum of 7 squares:

$$16 = 2^2 + 2^2 + 2^2 + 1^2 + 1^2 + 1^2 + 1^2$$

From the relations between the classes:

$$\begin{aligned} R^2 &= E & C_3^2 &= 2(E + R) \\ RC_3 &= C_3 & C_3C_3' &= C_3C_3'' = C_3' + C_3'' \\ RC_3' &= C_3'' & C_3C_4 &= 2C_4 \\ RC_3'' &= C_3' & C_3C_5 &= 2C_5 \\ RC_4 &= C_4 & C_3^2 &= C_3''^2 = 2E + C_3 \\ RC_5 &= C_5 & C_3'C_3'' &= 2R + C_3 \\ && C_3'C_4 &= C_3''C_4 = 2C_5 \\ && C_3'C_5 &= C_3''C_5 = 2C_4 \\ C_4^2 &= C_4^2 = 4E + 4R + 4C_3 \\ C_4C_5 &= 4C_3' + 4C_3'' \end{aligned}$$

there follows for the characters of the irreducible representations of the tetragonal double group the scheme of Table 7: The first 5 representations are the single-valued, the last two the double-valued representations of the tetragonal rotation group.

TABLE 7  
Characters of Tetragonal Double Group

	<i>E</i>	<i>R</i>	<i>C<sub>3</sub></i>	<i>C<sub>3'</sub></i>	<i>C<sub>3''</sub></i>	<i>C<sub>4</sub></i>	<i>C<sub>8</sub></i>
$\Gamma_1$	1	1	1	1	1	1	1
$\Gamma_2$	1	1	1	1	1	-1	-1
$\Gamma_3$	1	1	1	-1	-1	1	-1
$\Gamma_4$	1	1	1	-1	-1	-1	1
$\Gamma_5$	2	2	-2	0	0	0	0
$\Gamma_6$	2	-2	0	$\sqrt{2}$	$-\sqrt{2}$	0	0
$\Gamma_7$	2	-2	0	$-\sqrt{2}$	$\sqrt{2}$	0	0

We still have to reduce to irreducible components the double-valued representations of the spherical rotation group as representations of the tetragonal double group. The characters of the classes of the tetragonal double group in the  $(2j+1)$ -dimensional representation of the spherical rotation group are, by equation (4)

$$\chi = \frac{\sin(j + \frac{1}{2})\Phi}{\sin \frac{1}{2}\Phi} \quad (j + \frac{1}{2} = \text{integer}) \quad (2)$$

Angle of rotation	Character
$\Phi = 0$	$\chi_E = 2j + 1$
$\Phi = 2\pi$	$\chi_R = -(2j + 1)$
$\Phi = \pm\pi$	$\chi_3 = \chi_4 = \chi_8 = 0$
$\Phi = \pm\frac{\pi}{2}$	$\chi_{3'} = \frac{\sin\left(j + \frac{1}{2}\right)\frac{\pi}{2}}{\sin\frac{\pi}{4}} = \begin{cases} \sqrt{2}, & \text{for } j \equiv \frac{1}{2} \pmod{4} \\ 0, & \text{for } j \equiv \frac{3}{2}, \frac{1}{2} \pmod{4} \\ -\sqrt{2}, & \text{for } j \equiv \frac{1}{2} \pmod{4} \end{cases}$
$\Phi = \pm\frac{3\pi}{2}$	$\chi_{3''} = -\chi_{3'}$

The only essential values are  $\chi_E$  and  $\chi_{3'}$ . All other characters can be uniquely derived from these two, or else vanish. In detail one has:

TABLE 8

$j$	Characters of the classes in the reducible representation, i.e., in the $(2j+1)$ -dimensional representation of the spherical rotation group		Decomposition of the reducible representation into irreducible components
	$E$	$C_3'$	
$\frac{1}{2}$	2	$\sqrt{2}$	$\Gamma_6$
$\frac{3}{2}$	4	0	$\Gamma_6 + \Gamma_7$
$\frac{5}{2}$	6	$-\sqrt{2}$	$\Gamma_6 + 2\Gamma_7$
$\frac{7}{2}$	8	0	$2\Gamma_6 + 2\Gamma_7$
$4\lambda + j'$	$8\lambda + 2j' + 1$	as for $j'$	$2\lambda(\Gamma_6 + \Gamma_7)$ plus irreducible components for $j = j'$

### § 8. Double-Valued Representations of the Hexagonal and Cubic Symmetry Groups

a) Of the 6 classes of the simple hexagonal rotation group, three correspond to a rotation by  $\pm\pi$ , and consequently to one class each of the hexagonal double group; the other three ( $E$ ,  $C_3$ ,  $C_4$ ) contain rotations by  $0, \pm 2\pi/3, \pm\pi/3$ , and therefore correspond to two classes each of the double group. The double group accordingly contains 24 elements in 9 classes. Besides the 6 representations of the simple group there must accordingly exist three further representations of the double group; the sum of the squares of the dimensionalities of these representations must be equal to the number of new elements appearing in addition to those of the simple group, and thus must be 12; thus all three new representations (the double-valued representations of the simple hexagonal rotation group) are two-dimensional.

From the easily obtained relations between the classes, one finds the values shown in the following table for the characters of the individual classes of the hexagonal double group in the three newly added representations, which as representations of the simple group are double-valued (for the single-valued representations  $\Gamma_1$  to  $\Gamma_6$  of the simple group, see Table 3).

TABLE 9  
Double-Valued Representations of the Hexagonal Rotation Group

	$E$	$R$	$C_3$	$C_3'$	$C_3''$	$C_4'$	$C_4''$	$C_6$	$C_6$
$\Gamma_7$	2	-2	0	1	-1	$\sqrt{3}$	$-\sqrt{3}$	0	0
$\Gamma_8$	2	-2	0	1	-1	$-\sqrt{3}$	$\sqrt{3}$	0	0
$\Gamma_9$	2	-2	0	-2	2	0	0	0	0

In the  $(2j+1)$ -dimensional representation of the spherical rotation group the classes of the hexagonal double group have the following characters (Eq. (2)):

$$\begin{aligned} \chi_E &= 2j + 1 & \chi_R &= -\chi_E \\ \chi_2 &= \chi_3 = \chi_4 = 0 \\ \chi_3' &= \frac{\sin(2j+1)\frac{\pi}{3}}{\sin\frac{\pi}{3}} \left\{ \begin{array}{ll} 1, & \text{for } j \equiv \frac{1}{2} \pmod{3} \\ -1, & " \quad j \equiv \frac{2}{3} \pmod{3} \\ 0, & " \quad j \equiv \frac{1}{3} \pmod{3} \end{array} \right. \\ \chi_4' &= \frac{\sin(2j+1)\frac{\pi}{6}}{\sin\frac{\pi}{6}} \left\{ \begin{array}{ll} \sqrt{3}, & \text{for } j \equiv \frac{1}{2} \text{ or } \frac{4}{3} \pmod{6} \\ 0, & " \quad j \equiv \frac{2}{3} \text{ or } \frac{1}{3} \pmod{6} \\ -\sqrt{3}, & " \quad j \equiv \frac{1}{6} \text{ or } \frac{5}{6} \pmod{6} \end{array} \right. \\ \chi_3'' &= -\chi_3' & \chi_4'' &= -\chi_4'. \end{aligned}$$

From this, the decompositions of the double-valued representations of the spherical rotation group into irreducible representations of the hexagonal rotation group are found to be as follows:

TABLE 10

$j$	Decomposition into irreducible components
$\frac{1}{3}$	$\Gamma_1$
$\frac{2}{3}$	$\Gamma_1 + \Gamma_2$
$\frac{4}{3}$	$\Gamma_1 + \Gamma_2 + \Gamma_3$
$\frac{7}{3}$	$\Gamma_1 + 2\Gamma_2 + \Gamma_3$
$\frac{9}{3}$	$\Gamma_1 + 2\Gamma_2 + 2\Gamma_3$
$\frac{11}{3}$	$2\Gamma_1 + 2\Gamma_2 + 2\Gamma_3$
$6j + j'$	$2\lambda(\Gamma_1 + \Gamma_2 + \Gamma_3) + \text{decomposition for } j'$

b) The double octahedral group contains 48 elements in 8 classes, since the classes  $E$ ,  $C_3$ ,  $C_5$  of the simple octahedral group must each correspond to 2 classes of the double group. The octahedral group accordingly possesses three double-valued representations, comprising one four-dimensional and two two-dimensional representations ( $48 = 24 + 4^2 + 2^2 + 2^2$ , 24 being the sum of the squares of the dimensionalities of the single-valued representations). The characters of the individual classes of the double octahedral group in the double-valued representations of the octahedral group are:

TABLE 11

	$E$	$R$	$C_3$	$C_3'$	$C_3''$	$C_4$	$C_5'$	$C_5''$
$\Gamma_0$	2	-2	0	$\sqrt{2}$	$-\sqrt{2}$	0	1	-1
$\Gamma_1$	2	-2	0	$-\sqrt{2}$	$\sqrt{2}$	0	1	-1
$\Gamma_2$	4	-4	0	0	0	0	-1	1

In the  $(2j+1)$ -dimensional representation of the rotation group, we have

$$\begin{aligned} \chi_E &= 2j + 1 & \chi_R &= -\chi_E \\ \chi_3 &= \chi_4 = 0 \\ \chi_3' &= \frac{\sin(2j+1)\frac{\pi}{4}}{\sin\frac{\pi}{4}} = \begin{cases} \sqrt{2}, & \text{for } j \equiv \frac{1}{2} \pmod{4} \\ 0, & \text{" } j \equiv \frac{3}{2} \text{ or } \frac{7}{2} \pmod{4} \\ -\sqrt{2}, & \text{" } j \equiv \frac{5}{2} \pmod{4} \end{cases} \\ \chi_5' &= \frac{\sin(2j+1)\frac{\pi}{3}}{\sin\frac{\pi}{3}} = \begin{cases} 1, & \text{for } j \equiv \frac{1}{2} \pmod{3} \\ -1, & \text{" } j \equiv \frac{2}{3} \pmod{3} \\ 0, & \text{" } j \equiv \frac{4}{3} \pmod{3} \end{cases} \\ \chi_3'' &= -\chi_3' & \chi_5'' &= -\chi_5' \end{aligned}$$

TABLE 12  
Irreducible Components of the  $(2j+1)$ -Dimensional Double-Valued Representation of the Spherical Rotation Group when Reduced as Two-Dimensional Representation of the Octahedral Group

$j$	Irreducible components
$\frac{1}{2}$	$\Gamma_0$
$\frac{3}{2}$	$\Gamma_0$
$\frac{5}{2}$	$\Gamma_0 + \Gamma_1$
$\frac{7}{2}$	$\Gamma_0 + \Gamma_1 + \Gamma_2$
$\frac{9}{2}$	$\Gamma_0 + 2\Gamma_1$
$\frac{11}{2}$	$\Gamma_0 + \Gamma_1 + 2\Gamma_2$
$6 + j'$	$\Gamma_0 + \Gamma_1 + 2\Gamma_2$ + components for $j = j'$ with interchange of $\Gamma_0$ with $\Gamma_2$
$12l + j'$	$2\lambda(\Gamma_0 + \Gamma_1 + 2\Gamma_2)$ + components for $j = j'$

All angular momenta up to  $j = \frac{3}{2}$  are arbitrarily oriented in the cubic crystal; for larger angular momenta, the directional degeneracy is partly destroyed.

c) The rhombic rotation group possesses one double-valued irreducible representation:  $\chi_E = 2$ ,  $\chi_R = -2$ , and the characters of the rotations by  $\pi$  around the 3 axes are 0. The  $(2j+1)$ -dimensional double-valued representation of the spherical rotation group contains this irreducible representation  $j + \frac{1}{2}$  times.

## II. THE ZEROTH-ORDER EIGENFUNCTIONS IN THE CRYSTAL

### § 9. Eigenfunction of an Atom with Several Electrons

The eigenfunctions of a free atom with  $N$  electrons depend not only on the distances between the electrons and between electrons and nucleus, but also on the orientation of the entire system in space; but because of the spherical symmetry of the problem the  $2l + 1$  eigenfunctions that belong to a term with the azimuthal quantum number  $l$  are determined for all orientations of the system in space when they are given for one orientation. For example, we can, following Wigner<sup>1</sup>, assign the values of the functions arbitrarily on the  $(3N - 3)$ -dimensional

<sup>1</sup> E. Wigner, Ztschr. f. Phys. 43, p. 624, 640 (1927).

"hypersurface"  $x_1 = y_1 = x_2 = 0$ , as functions of the remaining coordinates of the electrons, and then the eigenfunctions can be found for any other orientation of the atom in space (any coordinates  $x_1, y_1, z_1$ ) by means of the  $(2l + 1)$ -dimensional representation of the rotation group. The assignment of the eigenfunctions on the hypersurface is of course "arbitrary" only to the extent that the behavior of the eigenfunctions under space rotations of the atom does not depend on the special choice of their values on the hypersurface; the actual eigenfunctions must of course be found by a detailed solution of the Schrödinger equation.

In the crystal, the behavior of the eigenfunctions is much less determined by the symmetry alone; they can be arbitrarily chosen not only on a  $(3N - 3)$ -dimensional hypersurface, but in a whole region of the  $3N$ -dimensional space, without coming into conflict with the transformation properties prescribed by the symmetry. If the position of the atomic nucleus in the crystal admits  $g$  symmetry operations, then the eigenfunctions of the atom can be arbitrarily chosen for all positions of the first electron inside a suitably chosen sector of solid angle  $\frac{4\pi}{g}$  through which no symmetry element passes, and for arbitrary positions of the other electrons. In the other  $g - 1$  regions of equal size, they are then determined in virtue of the group-theoretic representation of the symmetry operations of the crystal that is characteristic for the term in question. The exact determination of the eigenfunctions accordingly requires a much more thoroughgoing explicit solution of the Schrödinger equation than for the free atom.

But now, as is well known, it is an essential feature of the perturbation theory and it is indeed the perturbation of an atom on inclusion in the crystal that we want to study - that it requires first the specification of eigenfunctions of zeroth order; i.e., from the eigenfunctions of the unperturbed (spherically symmetric) problem one must choose precisely those onto which the eigenfunctions of the perturbed problem join continuously. Accordingly one proceeds as if one also knew completely the eigenfunctions of the atom in the crystal, if one prescribes them on Wigner's hypersurface, and uses the representation of the rotation group in the special form as reduced in terms of representations of the crystal group. Thus the symmetry operations of the crystal transform into each other only those eigenfunctions that belong to the same term of the atom in the crystal. But the general representation of the rotation group in the form reduced in terms of a crystal symmetry group would scarcely be simple. Therefore, we restrict ourselves to setting up the angle-dependent eigenfunctions in zeroth approximation for a single electron in the crystal, regarding its coupling with the other electrons of the atom as

suppressed. Such eigenfunctions will, however, be adequate in general also for the evaluation of exchange integrals in the crystal<sup>1</sup>, when one combines them with, say, the Hartree radial eigenfunctions, which indeed also hold for an uncoupled electron, and assumes that the inclusion of the atom in the crystal has no essential influence on the electron exchange inside an atom.

#### § 10. Zeroth-Order Eigenfunctions for an Uncoupled Electron in the Crystal

We first suppose that the Schrödinger equation for an electron of the free atom, considered as uncoupled from the other electrons, has been separated in polar coordinates; to the term with the azimuthal quantum number  $l$  there thus belong as angle-dependent eigenfunctions the surface harmonics of  $l$ th order. Then we attempt to use linear combinations of these spherical harmonics to get the correct zeroth-order eigenfunctions that belong to a definite term of the electron in the crystal, and that therefore transform under symmetry operations of the crystal atom according to a definite irreducible representation of the symmetry group of the crystal. We shall accordingly unite in a "society" all those spherical harmonics that transform among each other under symmetry operations of the crystal, and then by a suitable choice of linear combinations instead of the original spherical harmonics try to make these societies as small as possible - this corresponds to finding the irreducible representations. Finally there must correspond to every  $k$ -dimensional irreducible component of the  $(2l+1)$ -dimensional representation of the rotation group one irreducible society of  $k$  spherical harmonics of  $l$ th order. A society found in this way with a definite representation property for symmetry operations then comprises the correct zeroth-order eigenfunctions for the crystal term of just this representation property, if no further term of the same representation property arises from the same term of the unperturbed atom, i.e., if the  $(2l+1)$ -dimensional representation of the rotation group contains that particular irreducible representation of the crystal group only once. For the zeroth-order eigenfunctions  $\psi_i$  are to be determined by the requirement of the general perturbation theory:

$$\int V \psi_i \psi_k dx = 0, \quad i \neq k \quad (i = -l, \dots +l; \quad k = -l, \dots +l) \quad (3)$$

$V$  is the perturbation potential,  $x$  stands for all coordinates, and  $\psi_1$  and  $\psi_k$  are to transform under operations of the group of the crystal atom according to the

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<sup>1</sup>The search for such eigenfunctions was the starting point of the present work. Cf. also Ehrlert, Zeitschr. f. Phys., loc. cit.

transformations  $(a_{ij})$  and  $(b_{kl})$ . By Wigner's well-known argument one finds ( $g$  is the number of group elements, and  $R$  is a substitution of the group, under which  $V$  is accordingly unchanged):

$$\begin{aligned} \int V \psi_i(x) \psi_k(x) dx &= \frac{1}{g} \sum_R \int V(Rx) \psi_i(Rx) \psi_k(Rx) dx \\ &= \frac{1}{g} \sum_{j,l} \sum_R a_{ij}^R b_{kl}^R \int V \psi_j(x) \psi_l(x) dx \\ &= 0 \text{ for } a \neq b, \text{ i.e., for terms of different representations} \\ &= \delta_{ik} c_i, \quad \text{for } a = b \end{aligned} \tag{4}$$

Accordingly, if only one term belongs to a particular representation and if  $\psi_1$  is an eigenfunction for this term, then the integral vanishes both for such  $\psi_k$  as belong to other terms and for those that belong to the same term; thus the eigenfunctions  $\psi_1$  satisfy the requirement (3) of perturbation theory.

If on the other hand several ( $n$ ) terms belong to an irreducible representation, then in general the integral (3) does not vanish if by  $\psi_1$  and  $\psi_k$  one understands two eigenfunctions that belong to two different terms of the same representation. The  $n$  "societies" that belong to the same irreducible representation of the crystal group thus obviously do not in general as yet comprise the correct eigenfunctions of the problem, and these correct eigenfunctions cannot be determined at all by purely group-theoretical methods, but only by taking into account aspects of the particular problem in question. One must, as usual in perturbation theory, form from the  $nk$  spherical harmonics of the  $n$  societies  $nk$  new eigenfunctions  $\Psi_i$  by taking linear combinations:

$$\Psi_i = \sum_{j=1}^{nk} b_{ij} \psi_j \quad (i = 1, \dots, nk)$$

and determine the coefficients  $b_{ij}$  by solving the usual determinantal equation of degree  $nk$ . This equation gives for the term value  $nk$ -fold roots, and at the same time, one obtains the  $k$  zeroth-order eigenfunctions belonging to each. These eigenfunctions are not, however, linear combinations of spherical harmonics with universal coefficients; the coefficients depend on the detailed form of the electric field of the crystal. (The relative complication of this case, with several terms belonging to the same representation, is closely connected with the general theorem that terms of the same representation do not cross over each other (cf. § 22)). (An example is given in the next section).

### § 11. Eigenfunctions for Tetragonal and Hexagonal Symmetry

In order now actually to arrange the spherical harmonics into "societies" in such a way that under arbitrary symmetry operations of the crystal, the eigenfunctions of a society transform only among themselves, we consider each symmetry as a product of an interchange of the positive and negative directions of each axis and interchanges of the axes of the crystal with each other. Furthermore we write the spherical harmonics in real form,  $\sqrt{2} P_l^m (\cos \theta)^{\cos m\varphi}$ ; then under change of the directions of the axes every spherical harmonic changes at most its sign, and never goes over into another function. Accordingly, all that we have left to deal with is the interchange of different axes, and we see at once that in a rhombic crystal, every spherical harmonic written in real form makes up a society by itself, because interchanges of different axes do not belong to the group. Thus all eigenvalues are single, as we already showed by group-theoretical arguments.

For tetragonal-holohedral symmetry of the position of the atom, the two two-fold axes X and Y are interchangeable. This interchange carries<sup>1</sup>  $\cos \varphi$  over into  $\pm \sin \varphi$  and vice versa, and also carries  $\cos m\varphi$  over into  $\pm \sin m\varphi$  for all odd m, while for even m,  $\cos m\varphi$  at most changes its sign: For odd m,  $\cos m\varphi$  and  $\sin m\varphi$  belong to the same society, but for even m every function forms its own society.

Similarly, for the hexagonal-holohedral symmetry (the three two-fold axes perpendicular to the hexagonal axis are interchangeable)  $\cos m\varphi$  and  $\sin m\varphi$  belong to the same (two-fold) eigenvalue when m is not divisible by 3, and on the other hand they belong to two distinct single eigenvalues when m is a multiple of 3. In both cases, one obtains the number of distinct components known from the group-theoretical argument (§ 5).

But in both cases we can assert that our eigenfunctions are all correct ones only if the reduction of the  $(2l+1)$ -dimensional representation of the spherical rotation group in terms of the irreducible representations of the crystal group does not give any irreducible representation more than once. For tetragonal symmetry, this is the case for  $l \leq 2$ , for hexagonal symmetry for  $l \leq 3$ . For  $l = 3$ , on the other hand, with tetragonal symmetry, two terms belong to the same irreducible representation of the tetragonal group, namely the two-dimensional representation  $\Gamma_5$ . Thus in this case, of the eigenfunctions we have constructed, the only ones that are already the final correct eigenfunctions in zeroth approximation are those that correspond to a one-dimensional representation of the crystal group, i.e., that

<sup>1</sup>We of course identify the tetragonal axis Z with the axis of the spherical harmonics; moreover, we always use spherical harmonics with the normalization  $\int (P_l^m)^2 \sin \theta d\theta = 1$ .

form societies of one member. These are  $P_3^0$ ,  $\sqrt{2} P_3^1 \cos 2\varphi$  and  $\sqrt{2} P_3^1 \sin 2\varphi$ . The eigenfunctions belonging to the societies  $P_3^1$  and  $P_3^3$  are, on the other hand, not yet the final ones; one still has to form from them 4 linear combinations  $\psi_i$  ( $i = 1, 2, 3, 4$ ) that satisfy the condition

$$\int V \psi_i \psi_k d\tau = \delta_{ik} \varepsilon_i$$

of perturbation theory. In general, we write down the expression

$$\begin{aligned} \psi_i = & \psi_{ni}(r) (\alpha_{i1} \sqrt{2} P_3^1 \cos \varphi + \alpha_{i2} \sqrt{2} P_3^1 \sin \varphi \\ & + \alpha_{i3} \sqrt{2} P_3^3 \cos 3\varphi + \alpha_{i4} \sqrt{2} P_3^3 \sin 3\varphi) \end{aligned}$$

and get in the well-known way

$$\sum_{j=1}^4 \alpha_{ij} (\varepsilon_{jk} - \delta_{jk} \varepsilon_i) = 0 \quad k = 1, 2, 3, 4$$

where

$$\varepsilon_{jk} = \int V \psi_j \psi_k d\tau$$

$$\begin{aligned} \varepsilon_{11} &= 2 \int V \psi_{ni}^2(r) [P_3^1(\cos \theta)]^2 \cos^2 \varphi d\tau \\ &= 2 \int V \psi_{ni}^2 (P_3^1)^2 \sin^2 \varphi d\tau \\ &= \varepsilon_{22} = \int V \psi_{ni}^2 (P_3^1)^2 d\tau \\ \varepsilon_{33} &= \int V \psi_{ni}^2 (P_3^3)^2 d\tau = \varepsilon_{44} \\ \varepsilon_{13} &= \varepsilon_{31} = 2 \int V \psi_{ni}^2 P_3^1 P_3^3 \cos \varphi \cos 3\varphi d\tau \\ &= - 2 \int V \psi_{ni}^2 P_3^1 P_3^3 \sin \varphi \sin 3\varphi d\tau \\ &= - \varepsilon_{24} = - \varepsilon_{42} \end{aligned} \tag{5}$$

The relations come from the fact that  $V$ , the crystal potential, remains unchanged under a rotation by  $\pi/2$  around the  $Z$  axis. Furthermore it always follows from the invariance of  $V$  under reflection in the  $XZ$  plane (or rotation by  $\pi$  around  $X$ ) that all integrals vanish that contain products of  $\cos$  and  $\sin$ , e.g.,

$$\varepsilon_{14} = 2 \int V P_3^1 P_3^3 \psi_{ni}^2 \cos \varphi \sin 3\varphi d\tau = 0$$

Thus to determine the displacements of the terms, we have the determinantal equation

$$\begin{vmatrix} \epsilon_{11} - \epsilon & 0 & \epsilon_{13} & 0 \\ 0 & \epsilon_{11} - \epsilon & 0 & -\epsilon_{13} \\ \epsilon_{13} & 0 & \epsilon_{33} - \epsilon & 0 \\ 0 & -\epsilon_{13} & 0 & \epsilon_{33} - \epsilon \end{vmatrix} = [(\epsilon_{11} - \epsilon)(\epsilon_{33} - \epsilon) - \epsilon_{13}^2]^2 = 0$$

We obtain two eigenvalues

$$\epsilon', \epsilon'' = \frac{\epsilon_{11} + \epsilon_{33}}{2} \pm \sqrt{\left(\frac{\epsilon_{11} - \epsilon_{33}}{2}\right)^2 + \epsilon_{13}^2}$$

and as eigenfunctions for  $\epsilon'$

$$\begin{aligned} \psi_1' &= \sqrt{1 - \delta} P_3^1 \cos \varphi + \sqrt{1 + \delta} P_3^3 \cos 3\varphi \\ \psi_3' &= -\sqrt{1 - \delta} P_3^1 \sin \varphi + \sqrt{1 + \delta} P_3^3 \sin 3\varphi \end{aligned}$$

with

$$\delta = \frac{\epsilon_{13} - \epsilon_{11}}{\sqrt{(\epsilon_{33} - \epsilon_{11})^2 + 4\epsilon_{13}^2}}$$

and similarly as eigenfunctions for  $\epsilon''$

$$\begin{aligned} \psi_1'' &= \sqrt{1 + \delta} P_3^1 \cos \varphi - \sqrt{1 - \delta} P_3^3 \cos 3\varphi \\ \psi_3'' &= \sqrt{1 + \delta} P_3^1 \sin \varphi + \sqrt{1 - \delta} P_3^3 \sin 3\varphi \end{aligned}$$

In § 22, we shall prove that  $\epsilon_{13}$  actually does not vanish, so that  $\sqrt{2} P_3^1 \frac{\cos}{\sin} \varphi$  and  $\sqrt{2} P_3^3 \frac{\cos}{\sin} 3\varphi$ , are not yet the correct zeroth-order eigenfunctions, and furthermore that  $\epsilon_{13}$ , and so also  $\delta$ , and accordingly the zeroth-order eigenfunctions themselves, depend strongly on the special problem, in particular on the "orbit radius" of the electron and the departure of the symmetry from cubic symmetry.

For  $l > 3$  and tetragonal symmetry not only the two-dimensional, but also some of the one-dimensional irreducible representations into which  $(2l+1)$ -dimensional representation of the rotation group reduces have more than one term belonging to them, and it is more and more rarely that one can use the simple functions  $\sqrt{2} P_l^m \frac{\cos}{\sin} m\varphi$  as the zeroth-order eigenfunctions in the crystal. That is, with increasing azimuthal quantum number the splitting up in the tetragonal and also in the hexagonal crystal becomes more and more unlike the ordinary Stark-effect

TABLE 13  
Eigenfunctions for the Irreducible Representations of the  
Tetragonal and Hexagonal Rotation Group<sup>1</sup>

		Tetragonal				Hexagonal	
Representation with		Eigen-functions		Representation with		Eigen-functions	
Even λ	Odd λ			Even λ	Odd λ		
$\Gamma_1$	$\Gamma_3$	$P_0^4, \sqrt{2} P_1^{4\mu} \cos 4\mu\varphi$		$\Gamma_1$	$\Gamma_3$	$P_1^0, \sqrt{2} P_1^{6\mu} \cos 6\mu\varphi$	
$\Gamma_1$	$\Gamma_1$	$\sqrt{2} P_1^{4\mu} \sin 4\mu\varphi$		$\Gamma_1$	$\Gamma_1$	$\sqrt{2} P_1^{6\mu} \sin 6\mu\varphi$	
$\Gamma_3$	$\Gamma_4$	$\sqrt{2} P_1^{6\mu+2} \cos (4\mu+2)\varphi$		$\Gamma_3$	$\Gamma_4$	$\sqrt{2} P_1^{6\mu+8} \cos (6\mu+3)\varphi$	
$\Gamma_4$	$\Gamma_2$	$\sqrt{2} P_1^{6\mu+2} \sin (4\mu+2)\varphi$		$\Gamma_4$	$\Gamma_3$	$\sqrt{2} P_1^{6\mu+8} \sin (6\mu+3)\varphi$	
$\Gamma_6$	$\Gamma_6$	$\sqrt{2} P_1^{2\mu+1} \cos \sin (2\mu+1)\varphi$		$\Gamma_6$	$\Gamma_6$	$\sqrt{2} P_1^{6\mu \pm 2} \cos \sin (6\mu \pm 2)\varphi$	
				$\Gamma_6$	$\Gamma_6$	$\sqrt{2} P_1^{6\mu \pm 1} \cos \sin (6\mu \pm 1)\varphi$	

splitting in a homogeneous field, with which it agrees completely for  $l = 1$  (and for the hexagonal crystal also for  $l = 2$ ). The four-foldness or six-foldness of the principal axis manifests itself more and more, and causes departures from the relations that hold for an infinite-fold axis, which gives the symmetry relations for the Stark effect in a homogeneous field.

#### § 12. Eigenfunctions for Cubic (-Holohedral) Symmetry

For cubic-holohedral symmetry all three axes X, Y, Z are interchangeable. From this it follows at once that the three first-order spherical harmonics,  $P_1^0 = \sqrt{\frac{3}{2}} \cos \theta$  and  $\sqrt{\frac{3}{2}} \sin \theta \frac{\cos \varphi}{\sin \varphi}$ , are carried over into each other by symmetry operations of the cubic symmetry group: A P term is not split up (cf. § 4), the choice of the axis for the spherical harmonics is thus arbitrary, and the directional degeneracy of the angular momentum remains unchanged.

If we proceed to the D term, we see at once that by interchanges of the three crystal axes X, Y, Z the zonal spherical harmonic  $P_2^0 = \sqrt{\frac{5}{2}} \left[ \frac{3}{2} \cos^2 \theta - \frac{1}{2} \right]$  can only go over into a function that contains  $\cos \varphi$  (or  $\sin \varphi$ ) either not at all or to the second degree, that is, besides  $P_2^0$  itself only  $\sqrt{2} P_2^2 \cos 2\varphi = \sqrt{\frac{15}{8}} \sin^2 \theta \cdot (2 \cos^2 \varphi - 1)$ . If, for example, we replace the Z axis by the X axis,  $P_2^0$  goes over into

<sup>1</sup>These eigenfunctions are of course still not the "correct" zeroth-order eigenfunctions.

$$\begin{aligned} P_2^0(x) &= \sqrt{\frac{5}{2}} \left( \frac{3}{2} \sin^2 \vartheta \cos^2 \varphi - \frac{1}{2} \right) \\ &= -\frac{1}{2} P_2^0 + \frac{\sqrt{3}}{2} \sqrt{2} P_2^1 \cos 2\varphi \end{aligned}$$

Accordingly  $P_2^0$  and  $\sqrt{2} P_2^1 \cos 2\varphi$  belong to the same eigenvalue, which is two-fold degenerate. Similarly, interchanges of axes can only take

$$\sqrt{2} P_2^2 \sin 2\varphi = \sqrt{\frac{15}{2}} \sin \vartheta \cos \varphi \sin \vartheta \sin \varphi$$

over into such spherical harmonics as contain  $\cos \varphi$  or  $\sin \varphi$  (or both) only to the first degree, and thus, besides itself, only into

$$\sqrt{2} P_2^1 \cos \varphi \text{ and } \sqrt{2} P_2^1 \sin \varphi \quad (P_2^1 = \sqrt{\frac{15}{4}} \sin \vartheta \cos \vartheta)$$

We denote the two terms into which a D term splits up in a crystal with cubic symmetry by  $D_\gamma$  (two-fold term, representation  $\Gamma_3$ ) and  $D_\epsilon$  (three-fold term, representation  $\Gamma_5$ ). We present the corresponding eigenfunctions both in written-out form and also in Ehlert's<sup>1</sup> notation. In this notation

$$(\alpha \beta \gamma) = r^{l+1} \frac{\partial^l}{\partial x^\alpha \partial y^\beta \partial z^\gamma} \left( \frac{1}{r} \right), \quad l = \alpha + \beta + \gamma$$

Term	Rep	Eigenfunction, ordinary notation	Eigenfunction, Ehlert form
$D_\gamma$	$\Gamma_3$	$(2\gamma)_1 = \sqrt{\frac{5}{2}} \left( \frac{3}{2} \cos^2 \vartheta - \frac{1}{2} \right) = P_2^0$	(002)
		$(2\gamma)_2 = \sqrt{2} P_2^1 \cos 2\varphi = \sqrt{\frac{15}{8}} \sin^2 \vartheta \cos 2\varphi$	(200)–(020)
$D_\epsilon$	$\Gamma_5$	$(2\epsilon)_1 = \sqrt{2} P_2^2 \sin 2\varphi = \sqrt{\frac{15}{8}} \sin^2 \vartheta \sin 2\varphi$	(110)
		$(2\epsilon)_2 = \sqrt{2} P_2^1 \cos \varphi = \sqrt{\frac{15}{2}} \sin \vartheta \cos \vartheta \cos \varphi$	(101)
		$(2\epsilon)_3 = \sqrt{2} P_2^1 \sin \varphi = \sqrt{\frac{15}{2}} \sin \vartheta \cos \vartheta \sin \varphi$	(011)

<sup>1</sup> W. Ehlert, loc. cit.

In like fashion we obtain the eigenfunctions for the results of the splitting up of an F term in the crystal, by assigning to the same term the eigenfunctions that transform into each other on interchange of the axes.

Term	Rep.	Eigenfunction, ordinary notation	Eigenfunction, Ehlert form
$F_g$	$\Gamma_1$	$(3\beta) = \sqrt{2} P_3^1 \sin 2\varphi = \frac{\sqrt{210}}{4} \cos^3 \vartheta \sin^2 \vartheta \sin 2\varphi$	(111)
$F_g$	$\Gamma_4$	$(3\delta)_1 = P_3^2 = \sqrt{\frac{7}{2}} \left( \frac{5}{2} \cos^3 \vartheta - \frac{3}{2} \cos \vartheta \right)$	(003)
$F_g$	$\Gamma_4$	$(3\delta)_2 = \sqrt{2} \sqrt{\frac{5}{8}} P_3^3 \cos 3\varphi - \sqrt{2} \sqrt{\frac{3}{8}} P_3^1 \cos \varphi$	(300)
$F_g$	$\Gamma_4$	$(3\delta)_3 = \sqrt{2} \sqrt{\frac{5}{8}} P_3^3 \sin 3\varphi + \sqrt{2} \sqrt{\frac{3}{8}} P_3^1 \sin \varphi$	(030)
$F_g$	$\Gamma_8$	$(3\alpha)_1 = \sqrt{2} P_3^2 \cos 2\varphi$	(201) - (021)
$F_g$	$\Gamma_8$	$(3\alpha)_2 = \sqrt{2} \sqrt{\frac{3}{8}} P_3^3 \cos 3\varphi + \sqrt{2} \sqrt{\frac{5}{8}} P_3^1 \cos \varphi$	(120) - (102)
$F_g$	$\Gamma_8$	$(3\alpha)_3 = \sqrt{2} \sqrt{\frac{3}{8}} P_3^3 \sin 3\varphi - \sqrt{2} \sqrt{\frac{5}{8}} P_3^1 \sin \varphi$	(012) - (210)

Here as is well known

$$P_3^1 = \sqrt{\frac{21}{2}} \left( \frac{5}{4} \cos^3 \vartheta - \frac{1}{4} \right) \sin \vartheta$$

$$P_3^3 = \frac{\sqrt{70}}{8} \sin^3 \vartheta$$

Similarly for a G-term:

Term	Rep.	Eigenfunction, ordinary notation	Eigenfunction, Ehlert form
$G_g$	$\Gamma_1$	$(4\alpha) = \sqrt{\frac{7}{12}} P_4^0 + \sqrt{2} \sqrt{\frac{5}{12}} P_4^4 \cos 4\varphi$	(400) + (040) + (004)
$G_g$	$\Gamma_3$	$(4\gamma)_1 = \sqrt{2} P_4^3 \cos 2\varphi$	(400) - (040)
$G_g$	$\Gamma_3$	$(4\gamma)_2 = \sqrt{\frac{5}{12}} P_4^0 - \sqrt{2} \sqrt{\frac{7}{12}} P_4^4 \cos 4\varphi$	2 · (004) - (400) - (040)
$G_g$	$\Gamma_4$	$(4\delta)_1 = \sqrt{2} P_4^4 \sin 4\varphi$	(310) - (130)
$G_g$	$\Gamma_4$	$(4\delta)_2 = \sqrt{2} \sqrt{\frac{7}{8}} P_4^1 \cos \varphi - \sqrt{2} \sqrt{\frac{1}{8}} P_4^0 \cos 3\varphi$	(103) - (301)
$G_g$	$\Gamma_4$	$(4\delta)_3 = \sqrt{2} \sqrt{\frac{7}{8}} P_4^1 \sin \varphi + \sqrt{2} \sqrt{\frac{1}{8}} P_4^0 \sin 3\varphi$	(031) - (013)

Term	Rep.	Eigenfunction, ordinary notation	Eigenfunction, Ehler form
$G_5$	$T_5$	$(4\alpha)_1 = \sqrt{2} P_4^0 \sin 2\varphi$	(112)
		$(4\alpha)_2 = \sqrt{2} \sqrt{\frac{1}{8}} P_4^1 \cos \varphi + \sqrt{2} \sqrt{\frac{7}{8}} P_4^2 \cos 3\varphi$	(121)
		$(4\alpha)_3 = \sqrt{2} \sqrt{\frac{1}{8}} P_4^1 \sin \varphi - \sqrt{2} \sqrt{\frac{7}{8}} P_4^2 \sin 3\varphi$	(211)
		$P_4^0 = \sqrt{\frac{9}{2}} \left( \frac{35}{8} \cos^4 \vartheta - \frac{15}{4} \cos^2 \vartheta + \frac{3}{8} \right)$	
		$P_4^1 = \frac{3}{8} \sqrt{10} (7 \cos^3 \vartheta - 3 \cos \vartheta) \sin \vartheta$	
		$P_4^2 = \frac{3}{8} \sqrt{5} (7 \cos^3 \vartheta - 1) \sin^2 \vartheta$	
		$P_4^3 = \frac{3}{8} \sqrt{70} \cos \vartheta \sin^3 \vartheta$	
		$P_4^4 = \frac{3}{16} \sqrt{35} \sin^4 \vartheta$	

All our eigenfunctions are the correct zeroth-order eigenfunctions for the electron in the crystal atom, for two terms never belong to the same representation<sup>1</sup>. This would first occur in the splitting-up of an H term.

### § 13. Connection between the Splitting-Up of Terms and the Interpretation of Spherical Harmonics as Potentials of Multipoles

Every spherical harmonic of  $l$ th order gives the angular dependence of the potential of a multipole of the same order, as can most easily be seen from the Maxwell form of the spherical harmonics,

$$(\alpha\beta\gamma) = r^{l+1} \frac{\partial^l \left( \frac{1}{r} \right)}{\partial x^\alpha \partial y^\beta \partial z^\gamma}, \quad l = \alpha + \beta + \gamma$$

To every term of the electron for cubic symmetry there now corresponds a definite decomposition ("partition") of  $l$  into three summands  $\alpha, \beta, \gamma$ , as was already remarked by Ehler. Up to  $l = 3$  the converse of this statement also holds, which makes possible a quite intuitive interpretation of the splitting of terms for cubic symmetry:

For  $l = 1$  one gets three linearly independent eigenfunctions (100), (010), (001), which correspond to the potentials of dipoles oriented along the X, Y, and

<sup>1</sup>For Ehler's problem, the construction of the vibrational eigenfunctions of CH<sub>4</sub>, a further symmetrization is required, in which one has to form from the eigenfunctions belonging to the same term linear combinations with definite symmetry properties under interchange of the vertices of a tetrahedron.

$Z$  axes. These orientations of a dipole are obviously equally justified, and the three eigenfunctions belong to the same eigenvalue.

For  $l = 2$  we have

$$(200) + (020) + (002) = r^3 \Delta \frac{1}{r} = 0$$

Accordingly one gets:

a) The two linearly independent eigenfunctions  $(002)$  and  $(200) - (020)$ .

These correspond to the potentials of "stretched out" quadrupoles (Fig. 1a), i.e., quadrupoles consisting of oppositely directed dipoles separated along the direction of their axis. Since the directions  $X$ ,  $Y$ ,  $Z$  are equally justified, both eigenfunctions belong to the same two-fold eigenvalue  $D_y$ .

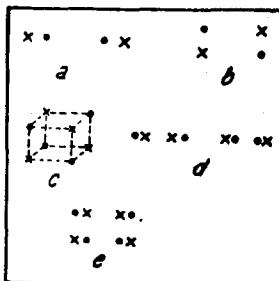


Fig. 1. Quadrupole and octupole classes for cubic symmetry.

b) The three linearly independent eigenfunctions  $(011)$ ,  $(101)$ ,  $(110)$  represent the potentials of surface-subtending quadrupoles, which consist of two dipoles separated perpendicularly to their axes (Fig. 1b). The three possible orientations of such a quadrupole in the  $YZ$ ,  $ZX$ , and  $XY$  planes, which correspond to the above potentials, are naturally equally justified, and the eigenfunctions belong to the same three-fold eigenvalue  $D_e$ .

For  $l = 3$  one gets:

a) The eigenfunction  $(111)$ , which represents the potential of a volume octupole (Fig. 1c), consisting of two equal and opposite surface-subtending quadrupoles separated perpendicularly to their planes. The eigenfunction belongs to the simple eigenvalue  $F_B$ .

b) The eigenfunctions  $(300)$ ,  $(030)$ ,  $(003)$ , which represent potentials of linearly extended octupoles (Fig. 1d), belong to the three-fold eigenvalue  $F_S$ .

c) The eigenfunctions  $(120) - (102)$ ,  $(012) - (210)$ ,  $(201) - (021)$ , potential functions of surface-wise extended octupoles<sup>1</sup>, which belong to the three-fold eigenvalue  $F_\epsilon$  (Fig. 1e).

For higher multipoles one has more complicated relations; see Ehrt's paper.

### III. THE ATOM UNDER THE INFLUENCE OF CRYSTALLINE FIELDS OF VARIOUS ORDERS OF MAGNITUDE

Hitherto we have dealt in general with the behavior of a quantum-mechanical system possessing a definite angular momentum in an electric field of prescribed symmetry. We must now discuss the three cases listed in the Introduction, which differ in the order of magnitude of the splitting of the terms in the crystal, and also correlate with each other the terms which one obtains in strong, intermediate, and weak crystalline fields.

#### § 14. The Angular Distribution of the Electron Density in a Strong Crystalline Field

In the first of the cases distinguished in the Introduction we can in first approximation neglect the exchange interaction of the electrons in the atom in question and assign a term value and an eigenfunction to the single electron. The actual term value is obtained by addition of the individual electron terms, and the eigenfunction by multiplication of the eigenfunctions of the electrons and "antisymmetrization" of the product<sup>2</sup>. (We speak of "eigenfunction of an individual electron", but are aware that all that can be prescribed is the form of the eigenfunction, the quantum cell, and that each electron in the atom has the same probability of being in this quantum cell).

The angular dependence of the eigenfunction of the individual electron is given in the free atom by some spherical harmonic of the  $l$ th order or by a linear combination of such functions, if  $l$  is the angular momentum of the "orbit" of the electron (cf. § 10). All  $2(2l + 1)$  quantum cells with the same  $l$  (and the same principal quantum number  $n$ ) belong to the same electron term value, and in the absence of the fixing of an axis by an external field it has no meaning to ask to which of the  $2(2l + 1)$  cells an electron belongs: Its probability for being present (density) depends only on the distance from the nucleus and does not prefer any direction in space; its "orbital plane" is arbitrary.

In the crystal, on the other hand, the shell consisting of  $2(2l + 1)$  quantum cells breaks up, according to the irreducible representations of the crystal symmetry

<sup>1</sup>The eigenfunctions  $(210) + (012) = -(030)$  and cyclic permutations are identical with those given under b).

<sup>2</sup>W. Heitler, Ztschr. f. Phys. Vol. 46, p. 47 (1928).

group, into several subshells, each corresponding to a different electronic term. If the splitting brought about by the crystalline field is sufficiently large or the temperature is sufficiently low, an individual electron will go into the subshell belonging to the lowest term, provided this is not yet "occupied". To every subshell, however, there belongs a quite definite angle-dependent eigenfunction, and the probability for the presence of the individual electron will therefore possess maxima in some directions in the crystal and vanish in others; the angular distribution of the electron density is a definite characteristic of each individual electron term in the crystal.

For example, a p electron in a tetragonal crystal will either go into the shell corresponding to the simple  $p_g$  term or into that corresponding to the two-fold term  $p_e$ , depending on the special form of the crystalline electric field (cf. § 22). In the former case the angular dependence of its density is given by  $\frac{3}{2} \cos^2\theta$ , so that the density has a maximum along the tetragonal axis ( $\theta = 0$ ) and vanishes in the plane of the two-fold axes. In the second case the density is proportional to  $\sin^2\theta$ , and accordingly shows the opposite behavior. If positive ions are located, say, close to the atom in question on the tetragonal axis and at greater distance perpendicular to it, the first case will correspond to a minimum of the energy, and vice versa.

The relationships are most interesting for cubic symmetry of the atom in the crystal. Here a p electron has no preferred orientation at all, all "places" in the p shell are energetically equivalent, and accordingly the probability for the presence of a p electron is in zeroth approximation distributed spherically around the nucleus. On the other hand a d electron can either occupy a place in the  $d_y$  subshell that includes four quantum cells - e.g., a d electron of a negative ion in a NaCl type crystal will always do this - or can go into the six-celled  $d_e$  shell, depending on which of the two crystal terms lies deeper. In the first case its eigenfunction will be  $P_1^0$  or with equal probability  $\sqrt{2} P_1^2 \cos 2\varphi$ , and its density will be given, apart from a factor depending on the distance from the nucleus, by

$$\rho = (P_1^0)^2 + 2(P_1^2)^2 \cos^2 2\varphi = \frac{1}{4}(\frac{3}{2} \cos^2\theta - \frac{1}{2})^2 + \frac{1}{4} \cdot \frac{1}{2} \sin^4\theta \cos^2 2\varphi \quad (7)$$

(The probabilities obtained from the two eigenfunctions are to be added) This density reaches a maximum  $\rho = 5/4$  on the three four-fold axes

$$\left( \theta = 0, \vartheta = \frac{\pi}{2}, \varphi = 0, \theta = \frac{\pi}{2}, \varphi = \frac{\pi}{2} \right)$$

and a minimum  $\rho = 0$  on the three-fold axes

$$\left( \cos \vartheta = \sqrt{\frac{1}{3}}, \vartheta = 54^\circ 44', \varphi = \frac{\pi}{4} \right)$$

Fig. 2 represents the density distribution graphically.

TABLE 14  
Density Distribution of a  $d_y$  Electron for Cubic Symmetry

$\theta$	$\varphi = 0$	10	20	30	40	45^\circ
0	1.25	1.25	1.25	1.25	1.25	1.25
10	1.14	1.14	1.14	1.14	1.14	1.14
20	0.87	0.87	0.87	0.86	0.86	0.86
30	0.55	0.54	0.52	0.50	0.49	0.49
40	0.37	0.35	0.30	0.25	0.22	0.21
50	0.34	0.31	0.21	0.10	0.03	0.02
60	0.61	0.55	0.39	0.21	0.10	0.08
70	0.92	0.83	0.61	0.36	0.20	0.18
80	1.16	1.06	0.80	0.50	0.31	0.28
90	1.25	1.14	0.86	0.55	0.34	0.31

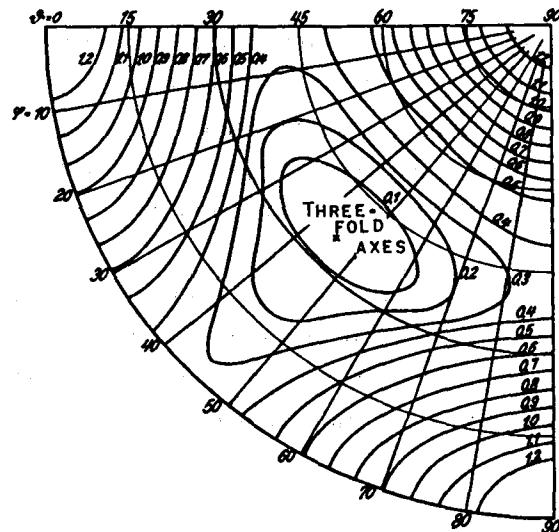


Fig. 2. Electron density distribution of the  $d_y$  electron for cubic symmetry.

If on the other hand the three-fold term  $d_2$  lies lower, then the electron density is greatest on the three-fold axes (diagonals of the cube).

This preference of the electron density for one axis of the crystal is already an effect of zeroth order, just as already in zeroth order the electrons of two hydrogen atoms that unite to form a molecule appear to be attracted to each other<sup>1</sup>. Here, as usual, the zeroth approximation means one that only selects the suitable ones from among the eigenfunctions of the unperturbed problem, without taking account of the perturbation of the eigenfunctions. When further approximations are carried through, of course no density function remains spherically symmetric, and the separation of the eigenfunction into the product of a radial factor and a spherical harmonic is then in general no longer legitimate. In these further approximations, there indeed does not occur any further splitting of the terms, but a further continuous displacement of the term value and deformation of the eigenfunction.

The total charge distribution of a closed shell is of course also no longer spherically symmetric when one calculates the higher approximations for the eigenfunction, i.e., takes into account the deformation by the crystalline field. But in zeroth approximation, the spherical symmetry of closed shells is retained, as also the total term value of a closed shell, in its property as a  $^1S$  term, can never show splitting.

#### § 15. Interaction of Electrons of Different Shells as Oriented in the Crystal

We now have the problem of correlating the terms that appear for the atom in the crystal with strong and intermediate values of the crystalline field (cases 1 and 2 of the Introduction). In both cases we begin with the prescription of the quantum numbers of the electrons that are not in closed shells, which we at first regard as not coupled to each other. In the case of the strong crystalline field we then have next to orient the angular momenta of the individual electrons with respect to the field (cf. preceding section), and then to study the interaction of the electrons while preserving their orientation. In the second case (intermediate crystalline field) we have to take into account the interaction in the free atom, i.e., first combine the orbital angular momenta of the electrons into the total orbital angular momentum  $\ell$  of the atom and then investigate the orientation of this angular momentum in the crystal. For intermediate crystal splitting, if there is no excitation, the ground state of the atom is at first definitely prescribed, and in the crystal the atom can always be only in a state that arises from the

<sup>1</sup>F. London, Ztschr. f. Phys. Vol. 46, p. 455 (1928).

ground state by Stark-effect splitting. In a strong crystalline field, on the other hand, each electron at first seeks for itself the lowest energy state; by interaction of the already oriented electrons an arbitrary term of the atom in the crystal can result, which by no means always needs to go over into the ground term of the free atom on removal of the crystalline field.

It is this state of affairs that we have to investigate group-theoretically. Let us take, say, two electrons with the azimuthal quantum numbers  $\ell$  and  $\lambda$ ; then the transformation of their eigenfunctions on rotation of the atom is given by the representations  $d_\ell$  and  $d_\lambda$  of the rotation group. In case 1 (strong crystalline field) we first carry out separately the reductions of  $d_\ell$  and  $d_\lambda$  as representations of the crystal symmetry group (orientation of the individual electron in the crystal); let

$$d_\ell = \sum \alpha_{lk} \gamma_k$$

$$d_\lambda = \sum \alpha_{ls} \gamma_s$$

The energy of the system composed of the two electrons is then for the present the sum of the energies of the individual electrons,  $E_k + E_\lambda$ ; the eigenfunction is to be taken as an antisymmetrized product of the eigenfunctions of the individual electrons and transforms under symmetry operations according to the representation  $\gamma_k \cdot \gamma_\lambda$  of the crystal group. Now we take into account the interaction of the two electrons for fixed orientation, i.e., for fixed terms of the individual electrons. Then the term  $E_k + E_\lambda$  splits up into several terms, which correspond to the irreducible components of  $\gamma_k \cdot \gamma_\lambda$ :

$$\gamma_k \cdot \gamma_\lambda = \sum \beta_{ks}^i T_i$$

**Case 2:** We first take into account the interaction of the electrons in the free atom, by making the reduction of  $d_\ell \cdot d_\lambda$  as a representation of the rotation group<sup>1</sup>:

$$d_\ell \cdot d_\lambda = \sum_{|\ell-\lambda|}^{|\ell+\lambda|} D_e$$

Then we insert the complete atom into the crystal and have to carry out the reduction of  $D_e$  as a representation of the crystal group:

<sup>1</sup>E. Wigner and J. v. Neumann, Ztschr. f. Phys. Vol. 49, p. 73. E. Fues, ibid. Vol. 51, p. 817 (1928).

$$D_e = \sum \alpha_e F_i$$

The order of succession of the group-theoretical reductions corresponds to the order of succession of the perturbation calculations, i.e., to the relative magnitudes of the contributions of the crystalline field and the electronic interaction to the term value. The number of final terms with a definite representation property must turn out the same by the two procedures. The correlation to each other of the individual terms for strong and intermediate crystalline fields can be obtained by the requirement that crystal terms of the entire atom which belong to the same representation of the symmetry group of the crystal must not cross over each other when one thinks of the crystalline field as increasing slowly from intermediate to high strength.

Example: In order to be free of the limitations of the Pauli principle, we investigate the terms of a system consisting of two d electrons with different principal quantum numbers  $n_1$  and  $n_2$  in a cubic crystal:

Case 1: Large splitting in the crystal.

a) Reduction of the representation of the rotation group belonging to the eigenfunction of the individual electron as a representation of the crystal group (cf. Table 2):

$$d_1 = \gamma_3 + \gamma_5$$

Without electronic interaction we obtain four terms: Both electrons can be in the state  $\gamma_3$ , or both in the state  $\gamma_5$ , or one in each state, in which last case, it is not a matter of indifference which is in the state  $\gamma_3$ , since the two electrons are distinguished by their principal quantum numbers. The terms without interaction correspond to the representations  $\gamma_3 \cdot \gamma_3$ ,  $\gamma_3 \cdot \gamma_5$ ,  $\gamma_5 \cdot \gamma_3$ , and  $\gamma_5 \cdot \gamma_5$  of the crystal group.

b) Inclusion of the interaction of the electrons, splitting up of each term in a) in accordance with the irreducible components of its representation<sup>1</sup>:

$$\gamma_3 \cdot \gamma_3 = \Gamma_1 + \Gamma_3 + \Gamma_5$$

$$\gamma_3 \cdot \gamma_5 = \Gamma_4 + \Gamma_6$$

$$\gamma_5 \cdot \gamma_3 = \Gamma_1 + \Gamma_3 + \Gamma_4 + \Gamma_6$$

<sup>1</sup>We denote the representation according to which the eigenfunctions of an individual electron transform by small Greek letters, that of the eigenfunction of the entire system by capital Greek letters.

## Case 2: Intermediate splitting in the crystal.

## a) Interaction of the electrons in the free atom:

$$d_2 \cdot d_2 = D_0 + D_1 + D_2 + D_3 + D_4$$

The free atom can be in an S, P, D, F, or G state; which of these is the lowest term can of course not be decided without exact calculation.

b) Orientation of the total orbital angular momentum in the crystal, reduction of that representation of the rotation group which corresponds to the term of the entire atom as representation of the octahedral group (Table 2):

$$D_0 = \Gamma_1$$

$$D_1 = \Gamma_4$$

$$D_2 = \Gamma_3 + \Gamma_5$$

$$D_3 = \Gamma_2 + \Gamma_4 + \Gamma_6$$

$$D_4 = \Gamma_1 + \Gamma_3 + \Gamma_4 + \Gamma_5$$

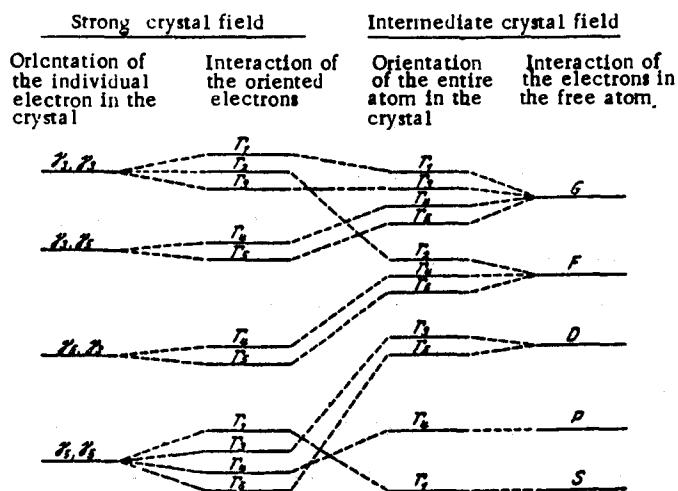


Fig. 3. Terms of a system of two d electrons with different principal quantum numbers, for cubic symmetry.

It is seen that we get, all told, the same terms as before. The correlation is shown in Fig. 3, for arbitrary assumptions about the relative positions of the terms.

### § 16. Interaction of Oriented Electrons of the Same Shell

In order to obtain only the terms allowed by the Pauli principle for a system of several electrons with the same principal and azimuthal quantum numbers, one proceeds most simply in a way analogous to that used for the corresponding problem in the free atom: One removes the remaining degeneracies wholly or partially, for cubic symmetry, say, by assuming one axis somewhat extended and thus reducing the symmetry to tetragonal; every degenerate term of a single electron in the cubic system thus splits up into terms of lower degeneracy in the tetragonal system, whose interaction can be treated simply. In this way one obtains the terms of the system of two electrons in a field of tetragonal symmetry, and then has to unite these into terms in the cubic field. The irreducible representations  $\Gamma_i$  of the octahedral group now contain, as one finds on using Tables 1, 5, 7, and 11 to obtain their reductions as representations of the tetragonal rotation group, the following irreducible components<sup>1</sup>:

$$\begin{array}{lll} \Gamma_1 = G_1 & \Gamma_4 = G_3 + G_5 & \Gamma_7 = G_6 \\ \Gamma_2 = G_3 & \Gamma_5 = G_4 + G_6 & \Gamma_8 = G_6 + G_7 \\ \Gamma_3 = G_1 + G_3 & \Gamma_6 = G_6 & \end{array}$$

It is useful to remove also the degeneracy of the two-fold term  $G_5$  of the tetragonal group, by again distinguishing one of the two-fold axes of the tetragonal symmetry group as against the other, and thus reducing the symmetry to the rhombic type. The reduction gives

$$G_1 = G_3 = \mathbb{G}_1 \quad G_3 = G_4 = \mathbb{G}_2 \quad G_6 = \mathbb{G}_3 + \mathbb{G}_4$$

The representations of the rhombic group are all one-dimensional, so that the product of two representations is again an irreducible representation:

$$\mathbb{G}_1 \mathbb{G}_1 = \mathbb{G}_1 \quad \mathbb{G}_1 \mathbb{G}_2 = \mathbb{G}_1 \quad \mathbb{G}_2 \mathbb{G}_3 = \mathbb{G}_4 \quad \mathbb{G}_3 \mathbb{G}_4 = \mathbb{G}_2 \quad \mathbb{G}_4 \mathbb{G}_2 = \mathbb{G}_3$$

As an example, we treat the interaction of two d electrons with the same principal quantum number, for cubic symmetry and strong crystalline field. The d shell first splits up into the  $\gamma_3$  ( $d_y$ ) subshell with 4 places (in counting the places we must include the two possible spin directions) and the  $\gamma_5$  subshell (term  $d_z^2$ ) with 6 places. If there is one electron in each subshell, then there arise by the interaction all the terms of the two-electron system having representations that are irreducible components of

<sup>1</sup>In this section we write representations of the cubic group with Greek, of the tetragonal group with Latin, and of the rhombic group with German letters.

$$\gamma_5 \gamma_5 = \Gamma_4 + \Gamma_8$$

and indeed always a triplet term and a singlet term, because the spin direction of the two electrons remains arbitrary on account of the different positional eigenfunctions. The total quantum weight of these terms is  $4 \cdot 6 = 24$ .

If, on the other hand, both electrons are in the  $\gamma_3$  subshell, then out of 16 modes of interaction only  $\frac{4 \cdot 3}{2} = 6$  are allowed. The representation properties of the terms of the system of two electrons are again given by the irreducible components of

$$\gamma_3 \gamma_3 = \Gamma_1 + \Gamma_2 + \Gamma_3$$

but the multiplicities of the individual terms are still unknown. As described above, we suppose the symmetry decreased to tetragonal; then the  $\gamma_3$  shell splits up into the  $g_1$  and  $g_3$  subshells of the tetragonal symmetry, with 2 places each. There is now only one way to get both electrons into the  $g_1$  subshell, namely if they have opposite spins. On the other hand, there are four possibilities for having one electron each in  $g_1$  and  $g_3$ , because then the spin is arbitrary. We get:

$$\begin{aligned} g_1 \cdot g_1 &= G_1 & \text{Quantum weight } 1 m_s &= 0 \\ g_1 \cdot g_3 &= G_3 & " & 4 m_s = -1001 \\ g_3 \cdot g_3 &= G_1 & " & 1 m_s = 0 \end{aligned}$$

This means three singlet terms with the representation properties  $G_1$ ,  $G_3$ ,  $G_1$  and one triplet term  $G_3$ . By comparison with (19) one sees that the term  $\Gamma_2$  of the two-electron system is a triplet and  $\Gamma_1$  and  $\Gamma_3$  are singlet terms.

We treat the interaction of two electrons in the cubic  $\gamma_5$  shell in the same way:

$$\gamma_5 \cdot \gamma_5 = \Gamma_1 + \Gamma_2 + \Gamma_4 + \Gamma_5 \quad \text{Quantum weight } \frac{6 \cdot 5}{2} = 15$$

Reduction to tetragonal symmetry yields:

$$\begin{aligned} \gamma_5 &= g_4 + g_5, \\ g_4 \cdot g_4 &= G_1 & \text{Quantum weight } 1 m_s &= 0 \\ g_4 \cdot g_5 &= G_5 & " & 8 m_s = -1001 \\ g_5 \cdot g_5 &= G_1 + G_2 + G_3 + G_4 & " & 6 m_s = ? \end{aligned}$$

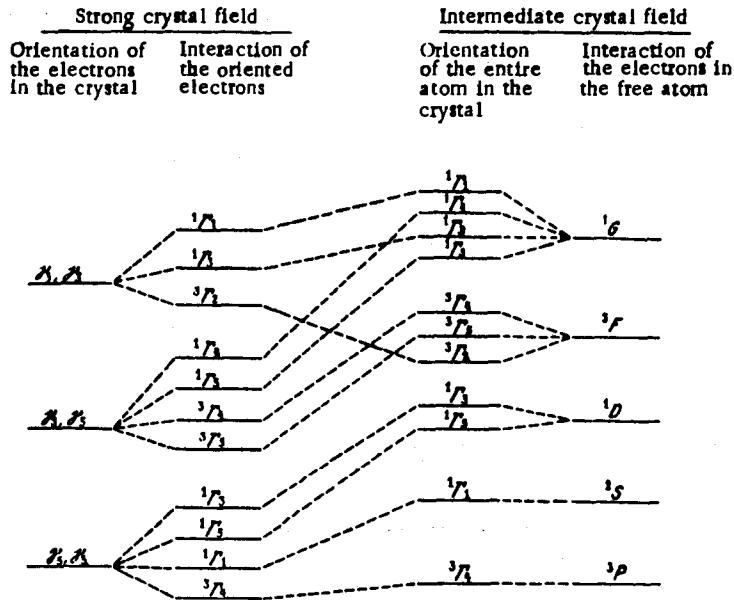


Fig. 4. Terms of a system of two d electrons of the same principal quantum number, for cubic symmetry.

Further reduction to rhombic symmetry yields:

$$\begin{aligned}
 g_5 &= g_3 + g_4 \\
 g_3 \cdot g_3 &= G_1 \quad \text{Quantum weight } 1 \quad m_s = 0 \\
 g_3 \cdot g_4 &= G_2 \quad " \quad 4 \quad m_s = -1001 \\
 g_4 \cdot g_4 &= G_1 \quad " \quad 1 \quad m_s = 0
 \end{aligned}$$

Combination into two-electron terms for tetragonal symmetry yields:

$$g_5 g_5 = ^1G_1 + ^1G_2 + ^1G_3 + ^1G_4 \quad \text{or} \quad ^1G_1 + ^3G_2 + ^1G_3 + ^1G_4$$

Combination into terms for cubic symmetry yields:

$$\gamma_5 \gamma_5 = ^1T_1 + ^1T_3 + ^1T_4 + ^3T_5 \quad \text{or} \quad ^1T_1 + ^1T_3 + ^3T_4 + ^1T_5$$

Whether  $T_4$  or  $T_5$  is the triplet term depends on the azimuthal quantum number  $l$  of the two  $\gamma_5$  electrons; in our case  $l = 2$ ,  $T_5$  is the triplet term.

The correlation of the terms of the quantum-mechanical system composed of two d electrons can be seen from Fig. 4, for arbitrary assumptions about the positions of the terms.

The interaction of more than two electrons oriented in the crystal can be treated in exactly the same way, and the correlation of the terms in the "strong" and "intermediate" crystalline fields can be completely carried through. We give the representation properties of the crystal terms that can arise from the interaction of several electrons of the same subshell, for cubic symmetry:

TABLE 15

Number of Electrons	Subshell $\gamma_3$	Subshell $\gamma_4$	Subshell $\gamma_5$
1	$^4F_3$	$^4F_4$	$^4F_5$
2	$^1F_1 + ^3F_3 + ^1I_5$	$\left\{ \begin{array}{l} ^1I_1 + ^1F_3 + ^1F_4 + ^1F_5 \\ ^1I_1 + ^1F_3 + ^3F_4 + ^1I_5 \end{array} \right\}$	as $\gamma_4$
3	$^4F_3$	$\left\{ \begin{array}{l} ^1F_1 + ^3F_3 + ^1F_4 + ^1F_5 \\ ^1F_1 + ^3F_3 + ^3F_4 + ^1F_5 \end{array} \right\}$	$^4F_5 + ^3F_5 + ^1F_5$
4	$^1F_1$	as for 2 electrons in the shell	
5	—	$^3F_1$	$^3F_1$
6	—	$^1F_1$	$^1F_1$

### § 17 Interaction between Orbital Angular Momentum and Spin

Let an atom be described by its orbital angular momentum  $\ell$  and the total spin  $s$  (term multiplicity  $2s + 1$ ). That is, under a common rotation of all electron positions around the nucleus, with spin direction preserved, the wave function of the atom transforms according to the representation  $D_\ell$  of the rotation group; under rotation of the spin direction alone, it transforms according to the representation  $D_s$ .<sup>1</sup>

In case 2 of the Introduction (Stark-effect splitting in the crystal large in comparison with the multiplet splitting) the orbital angular momentum  $\ell$  orients itself independently in the crystal; the entire multiplet is to be taken as the original state and splits up in the crystal into Stark-effect components that correspond to the irreducible components  $\Gamma_\lambda$  of the representation  $D_\ell$  of the spherical rotation group:

$$D_\ell = \sum \alpha_{\ell\lambda} \Gamma_\lambda$$

Each of these Stark-effect components now splits up further by the interaction with the spin:

<sup>1</sup>The first rotation corresponds to the transformation  $P_M$  of Wigner and von Neumann, loc. cit., the second to the transformation  $Q_M$ .

$$\Gamma_1 D_s = \sum a_{l\mu} F_\mu$$

This further splitting is of the order of magnitude of the multiplet splitting, but the number of components of a term  $\Gamma_\lambda$  is in general not equal to  $2s + 1$ .

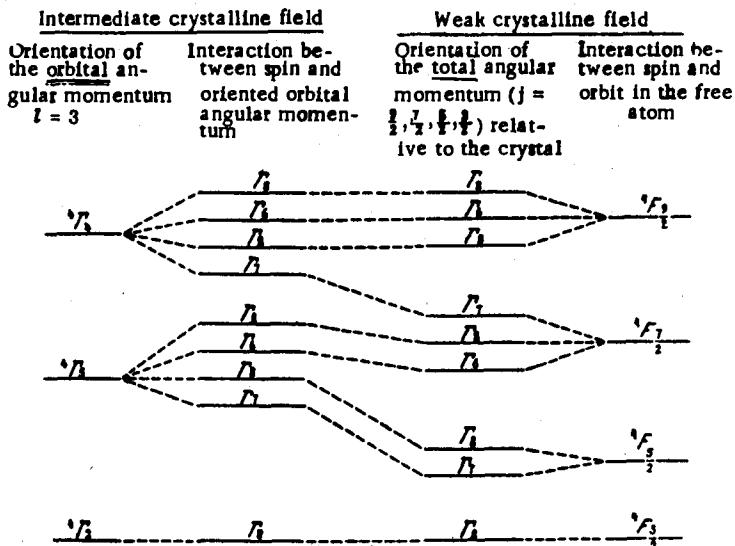


Fig. 5. Orientation of an atom in a  $^4F$  state in intermediate and weak fields of cubic symmetry.

In case 3 (crystal splitting small in comparison with multiplet splitting) the spin and orbital angular momentum first combine into the total angular momentum  $j$  of the atom:

$$D_l D_s = \sum_{|l-s|}^{l+s} D_j$$

and this orients itself relative to the crystal axes:

$$D_j = \sum a_{j\mu} F_\mu$$

i.e., each multiplet individually undergoes in the crystal a further splitting-up of smaller size than the multiplet splitting. Fig. 5 shows the splitting of a

<sup>4</sup>F term for cubic symmetry in intermediate and weak crystalline fields.<sup>1</sup>

#### IV. MAGNITUDE OF THE SPLITTING

##### § 18. General Formula for the Term of an Electron in an Ionic Crystal

After having so far oriented ourselves in a qualitative way about the Stark effect in a crystal, we now wish to calculate also the magnitude of the splitting, at least for the case of the strong crystalline field (every electron with its own term value). It turns out that quite generally the Stark effect in the inhomogeneous field of the crystal is formally an effect of first order, in contrast with the Stark effect in a homogeneous field, for which the first-order perturbation energy always vanishes. Suppose that only one of the terms that arise in the crystalline field from the term  $(n, l)$  of the electron in the free atom belongs to the representation  $\Gamma_\lambda$  of the crystal group. Then the position of this term  $\lambda$  relative to that of the unperturbed atom is

$$E_i = - \int e V \psi_{nli}^2 d\tau \quad (8)$$

Here  $V_e$  is the potential energy of the electron in the field of the other atom of the crystal, and  $\psi_{nli}$  is an arbitrary one of the zeroth-order eigenfunctions belonging to the term  $(n, l, \lambda)$ .  $\psi_{nli}$  can be written as the product of a radial factor and a linear combination of spherical harmonics:

$$\psi_{nli} = \psi_{nl} \sum_{m=0}^l c_{lm} P_l^m(\cos \vartheta) \frac{\cos m\varphi}{\sin m\varphi} \quad (9)$$

Accordingly we need integrals of the form

$$K'_{m\mu} = - \int V e \psi_{nli}^2(r) P_l^m(\cos \vartheta) P_l^\mu(\cos \vartheta) \frac{\cos m\varphi}{\sin m\varphi} \frac{\cos \mu\varphi}{\sin \mu\varphi} d\tau \quad (10)$$

By means of such integrals we can evidently also determine all the term values when several terms belong to the same representation of the crystal group (§ 10, 11) and to calculate the eigenvalues one has to set up a special perturbation calculation in which the matrix elements

<sup>1</sup>In practice transitional conditions between intermediate and strong fields (or between intermediate and weak) are probably of most frequent occurrence.

$$\epsilon_{ll} = - \int V e \psi_{nl}^2 d\tau,$$

$$\epsilon_{lk} = - \int V e \psi_{nl} \psi_{nk} d\tau$$

are involved.

If there is at least symmetry of the rhombic-holohedral type, all of the integrals  $K_{m\mu}$  that contain  $\cos m\varphi$  and  $\sin \mu\varphi$  mixed vanish. For under reflection in the XZ plane  $V$  is unchanged, whereas  $\cos m\varphi$   $\sin \mu\varphi$  takes the opposite sign, but the integral  $K_{m\mu}$  must be invariant under such changes of the variables of integration, and thus must vanish. We now write:

$$K_{m\mu}^{co} = - \int V e \psi_{nl}^2(r) P_l^m(\cos \theta) P_l^\mu(\cos \theta) \cos m\varphi \cos \mu\varphi d\tau$$

$$= - \frac{1}{2} \int V e \psi_{nl}^2 P_l^m P_l^\mu [\cos(m-\mu)\varphi + \cos(m+\mu)\varphi]$$

$$K_{m\mu}^{do} = - \frac{1}{2} \int V e \psi_{nl}^2 P_l^m P_l^\mu [\cos(m-\mu)\varphi - \cos(m+\mu)\varphi]$$

If we rotate the coordinate system by  $\pi$  around the Z axis,  $V$  is unchanged, but for odd  $m \pm \mu$ ,  $\cos(m \pm \mu)\varphi$  changes its sign, so that

$$\int V e \psi_{nl}^2 P_l^m P_l^\mu \cos(m \pm \mu)\varphi d\tau = 0, \quad m \pm \mu \text{ odd}$$

We now specialize from rhombic to tetrahedral symmetry. Then  $V$  also remains unchanged under rotations by  $\pi/2$  around Z, while  $\cos(m \pm \mu)\varphi$  changes its sign on this rotation if  $\frac{m \pm \mu}{2}$  is odd. Accordingly there remain different from zero for tetragonal, and naturally also for cubic, symmetry only the integrals

$$K_{m\mu} = - \int V e \psi_{nl}^2 P_l^m P_l^\mu \cos 4\sigma\varphi d\tau \quad (4\sigma = m \pm \mu) \quad (10a)$$

and analogously for hexagonal symmetry

$$K_{m\mu} = - \int V e \psi_{nl}^2 P_l^m P_l^\mu \cos 6\sigma\varphi d\tau \quad (6\sigma = m \pm \mu) \quad (10b)$$

We now assume that we have before us an ionic crystal, and write the potential  $V$  as the sum of the potentials arising from all ions except the particular one under consideration (perturbing potential):

$$V = \sum_i \frac{l_i}{r_i} \quad (11)$$

We locate the origin of our system of polar coordinates at the nucleus of the ion under consideration; let the coordinates of the  $i$ th ion (source ion) be  $R_i, \Theta, \Phi$ , and those of the argument of  $V$  be  $r, \theta, \varphi$ ; the angle between the radii vectores from the nucleus of the ion under consideration to these points is  $\alpha$ , and  $r_i$  is the distance from the source ion to the argument of  $V$ .

We develop the potential produced by the  $i$ th ion in spherical harmonics, with the normalization customary in quantum mechanics [ $\int (P_l^m)^2 \sin \theta d\theta = 1$ ]:

$$\frac{1}{r_i} = \sum_{s=0}^{\infty} \frac{r'}{R_i^{s+1}} \sqrt{\frac{2}{2s+1}} P_s^0(\cos \alpha)$$

By the definition of  $\alpha$  we have from the addition theorem of spherical harmonics

$$\frac{1}{r_i} = \sum_{s=0}^{\infty} \frac{r'}{R_i^{s+1}} \frac{2}{2s+1} \sum_{e=-s}^{+s} P_s^e(\cos \Theta) P_s^e(\cos \vartheta) e^{ie(\theta-\varphi)}$$

and the contribution of the  $i$ th ion to the integral  $K_{m\mu}$  becomes

$$\begin{aligned} K'_{m\mu} &= -ee_i \int \psi_{n1}^2(r) r^2 dr \sum_{s=0}^{\infty} \frac{r'}{R_i^{s+1}} \cdot \frac{2}{2s+1} \sum_{e=-s}^{+s} P_s^e(\cos \Theta) \\ &\times \int_0^{2\pi} \sin \vartheta d\vartheta P_s^e(\cos \vartheta) P_i^m(\cos \vartheta) P_i^\mu(\cos \vartheta) \\ &\times \int_0^{2\pi} d\varphi \cos 4\sigma \varphi (\cos \rho \varphi \cos \rho \Phi + \sin \rho \varphi \sin \rho \Phi) = -ee_i \\ &\times \int \psi_{n1}^2(r^2) dr \sum_{s=0}^{\infty} \frac{r'}{R_i^{s+1}} \sqrt{\frac{2}{2s+1}} P_s^{4\sigma}(\cos \Theta) \cos 4\sigma \Phi \cdot \alpha_{lm\mu}^{se} \end{aligned}$$

where

$$\alpha_{lm\mu}^{se} = \sqrt{\frac{2}{2s+1}} \int P_s^{4\sigma} P_i^m P_i^\mu \sin \vartheta d\vartheta \quad (12)$$

is the "expansion coefficient" of the product of spherical harmonics,  $P_l^m P_l^\mu$ , with respect to the spherical harmonic  $P_s^{4\sigma}$ . This quantity  $\alpha$  can be regarded as a multipole moment of the  $s$ th order of the "transition function"  $P_l^m P_l^\mu$ ; it is a numerical factor of the order of magnitude 1 (cf. § 19).

We now have

$$K_{m\mu}^l = -ee_i \sum_{s,\sigma} \frac{P_s^{4\sigma}(\cos \theta) \cos 4\sigma \Phi}{R_i^{s+1}} \bar{r}^s \alpha_{lm\mu}^{s\sigma}$$

where

$$\bar{r}^s = \int r^s \psi_{nl}^2(r) r^s dr$$

is the mean value of the  $s$ th power of the distance of the electron from the nucleus of the atom, accordingly a trifle more than the  $s$ th power of the "orbit radius" of the electron. The contribution of the moment of  $s$ th order to  $K_{m\mu}^l$  is accordingly proportional to, say,

$$\frac{e^s}{R_i} \cdot \frac{\bar{r}^s}{R_i^{s+1}} \approx (\text{Lattice energy}) \cdot \left( \frac{\text{Radius of electron orbit}}{\text{Distance of source ion from ion in question}} \right)^s$$

Since, however, the orbit radius will scarcely be greater than one-fourth of the lattice spacing, the higher moments contribute only very little to  $K_{m\mu}^l$ , and we can limit ourselves to the consideration of small values of  $s$ . But now  $s \geq 4\sigma$ , so that only  $\sigma = 0$  or 1 will be of interest for the calculation of the terms.

A.  $\underline{\sigma = 0}$ . According to Eq. (10a) such integrals occur only when  $m = \mu$ , and thus always have the form  $\int V e \psi_{nl}^2 (P_l^m)^2 dw$ . The consideration of such integrals alone is sufficient, for example, for the calculation of the values of the terms that arise with cubic symmetry from a d or an f term. We at once get

$$K_{mm}^l = -ee_i \sum_{s=0}^{\infty} \frac{P_s^0(\cos \theta)}{R_i^{s+1}} \bar{r}^s \cdot \alpha_{lm\mu}^{s0}$$

According to the definition of the spherical harmonics one has

$$\frac{P_l^m(\cos \theta)}{R_l^{s+1}} = \frac{1}{s!} \left( \frac{\partial^s}{\partial z^s} \right)_{\theta=0} x - y - z = 0$$

and accordingly when one sums over the contributions of all ions  $i$

$$K_{nm} = -e \int V \psi_{nl}^2(r) [P_l^m(\cos \theta)]^s d\tau = -e \sum_{s=0}^{\infty} \vec{r} \cdot \frac{1}{s!} \left( \frac{\partial^s V}{\partial z^s} \right)_0 \alpha'_{lm}$$

Here one has

$$\alpha'_{lm} = \alpha'_{lmn} = \int P_l^m(P_l^m)^s \sin \theta d\theta \quad (12a)$$

For  $s = 0$  and  $\alpha'_{lm} = 1$ ,  $\vec{r}^0 = 1$ , so that

$$K_{nm} = -e V_0 - e \sum_{s=1}^{\infty} \vec{r} \cdot \frac{1}{s!} \left( \frac{\partial^s V}{\partial z^s} \right)_0 \cdot \alpha'_{lm}$$

$-eV_0$  is the potential energy that the electron would possess if it were concentrated at the nucleus of the ion under consideration. But now the center of gravity of all the terms that arise in the crystal from one term of the free atom is displaced relative to the term of the free atom by precisely the amount

$$E_0 = -\frac{e}{2l+1} \int V \psi_{nl}^2(r) \sum_l (P_{ll})^s d\tau = -eV_0$$

for the zeroth-order density functions  $\psi_{nl}^2(r) P_l^2 \lambda$  that belong to the individual crystal terms ( $n, l$ ) combine according to the addition theorem of the spherical harmonics to form the spherically symmetric electron density  $(2l+1)\psi_{nl}^2(r)$  of the closed shell, and the integration of  $V$  over a spherical shell then gives the potential  $V_0$  at the position of the nucleus.

A term of the electron in the crystal atom with the eigenfunction  $\psi_{nl}(r) P_l^m(\cos \theta) e^{\pm im\phi}$  thus has the position, relative to the center of gravity of all crystal terms with the same principal quantum number  $n$  and azimuthal quantum number  $l$ , given by

$$E_n = K_{nn} - E_0 = -e \sum_{s=1}^{\infty} \vec{r} \cdot \frac{1}{s!} \left( \frac{\partial^s V}{\partial r^s} \right)_0 \alpha_{ns}^s \quad (14)$$

As has been said, the main contribution to this expression (14) is made by the first terms of the series. Every term is the product of three independent factors:

1. The mean value of the  $s$ th power of the distance of the electron from the nucleus.
2. The  $s$ th derivative of the lattice potential  $V$  at the position of the nucleus of the ion in question.
3. The intrinsic splitting factor  $\alpha_{lm}^s$  (multipole moment of the electron density).

B.  $\sigma = 1$ . Sums of the form (10c) with  $\sigma = 1$  occur in the calculation of the following integrals (cf. Eq. (10a)):

$$\begin{aligned} & -e \int V \psi_{nl}^s [P_l^2(\cos \vartheta)]^s (\cos^2 2\varphi - \sin^2 2\varphi) d\tau \\ & \qquad \qquad \qquad (2+2=4) \\ & -e \int V \psi_{nl}^s P_l^1(\cos \vartheta) P_l^3(\cos \vartheta) \cos \varphi \cos 3\varphi d\tau \\ & \qquad \qquad \qquad (1+3=4) \\ & -e \int V \psi_{nl}^s P_l^{m+2} P_l^{m-2} \cos(m+2)\varphi \cos(m-2)\varphi d\tau \\ & \qquad \qquad \qquad ((m+2)-(m-2)=4) \end{aligned}$$

The first type of integral, for example, determines the separation of the two terms with the eigenfunctions  $\sqrt{2} P_l^2 \cos 2\varphi$  and  $\sqrt{2} P_l^2 \sin 2\varphi$  for tetragonal symmetry, and the two other types occur primarily when several terms belong to the same representation (cf. the matrix element  $\epsilon_{1g}$  in § 11, also § 22).

The only important summand in Eq. (10c) is in this case the term with  $s = 4$  (because of the falling off of the terms with increasing  $s$ ). For this term we have:

$$\begin{aligned} \sqrt{\frac{2}{9}} P_4^4 &= \sqrt{\frac{35}{128}} \sin^4 \vartheta \\ \frac{1}{E_i^4} \sqrt{\frac{35}{128}} \sin^4 \theta \cos 4\Phi &= \frac{1}{16} \cdot \frac{1}{4!} \left( 4 \frac{\partial^4}{\partial x^4} + 4 \frac{\partial^4}{\partial y^4} - 3 \frac{\partial^4}{\partial z^4} \right) \frac{1}{R} \end{aligned}$$

Furthermore, in view of the tetragonal symmetry,

$$\frac{\partial^4 V}{\partial x^4} = \frac{\partial^4 V}{\partial y^4}$$

$$K_{\mu\mu} = -e \cdot \frac{1}{4!} \cdot \frac{1}{16} \left( 8 \frac{\partial^4 V}{\partial x^4} - 3 \frac{\partial^4 V}{\partial z^4} \right) r^{-4} \int \sin^4 \theta P_l^m P_l^{\mu} \sin \theta d\theta + \text{terms of higher order} \quad (15)$$

For cubic or nearly cubic symmetry we have also

$$\frac{\partial^4 V}{\partial x^4} = \frac{\partial^4 V}{\partial z^4}$$

$$K_{\mu\mu} = -e \cdot \frac{1}{4!} \cdot \frac{5}{16} \frac{\partial^4 V}{\partial z^4} r^{-4} \int \sin^4 \theta P_l^m P_l^{\mu} \sin \theta d\theta + \text{terms of higher order} \quad (15a)$$

For hexagonal symmetry 6 must be written everywhere instead of 4, and thus the integrals with  $\sigma = 0$  (cf. A) are at most to be corrected by contributions of multipole moments of 6th order.

#### § 19. Expansion of Squares and Products of Spherical Harmonics in Terms of Spherical Harmonics

We are interested in the expansion coefficients of squares of spherical harmonics in terms of zonal harmonics:

$$\alpha'_{lm} = \sqrt{\frac{2}{2s+1}} \int P_s^0 (P_l^m)^2 \sin \theta d\theta \quad (12a)$$

and also in the following expansion coefficients in terms of the harmonics  $P_4^l$ :

$$\begin{aligned} \beta_{lm} &= \int \sin^4 \theta (P_l^m)^3 \sin \theta d\theta \quad \text{for } m = 2 \\ \beta'_{lm} &= \int \sin^4 \theta P_l^{m-1} P_l^{m+1} \sin \theta d\theta \quad \text{for } m = 2 \\ \beta''_{lm} &= \int \sin^4 \theta P_l^{m-2} P_l^{m+2} \sin \theta d\theta \quad \text{for } m > 2 \end{aligned} \quad (16)$$

which occur in Eqs. (14) and (15).

We begin with  $\alpha'_{lm}$ : Since  $[P_l^m(\cos \theta)]^2$  is a polynomial in  $\cos \theta$  of degree  $2l$ , it can be expanded in terms of the first  $2l$  zonal harmonics alone:

$$\alpha'_{lm} = 0 \text{ for } s > 2l$$

That is, the electron density distribution has no higher multipoles than those of  $(2l)$ th order, and our series (14) for the calculation of the terms in the crystal is always finite. In addition all expansion coefficients with odd index  $s$  vanish, because  $(P_l^m)^2$  is an even function of  $\cos \theta$ . There remain to be calculated

$$\alpha_{lm}^s \text{ for } s = 2\sigma, 0 \leq \sigma \leq l$$

Here we are primarily interested in the expansion coefficients with small  $s$ , which we calculate by the method used by Sommerfeld<sup>1</sup> for the normalization of the spherical harmonics. Accordingly we replace one factor  $P_l^m(x)$  by the differential expression

$$P_l^m(x) = \sqrt{\frac{l-m!}{l+m!}} \cdot \frac{2l+1}{2} \cdot \frac{(1-x^2)^{m/2}}{2^l \cdot l!} \cdot \frac{d^{l+m}}{dx^{l+m}} \cdot (x^2 - 1)^l$$

and write the other as a polynomial in  $x$ , in which we need the two highest powers (the others disappear in differentiations later on)

$$P_l^m(x) = \sqrt{\frac{l-m!}{l+m!}} \cdot \frac{2l+1}{2} \cdot \frac{2l!}{2^l \cdot l! \cdot l-m!} \cdot (1-x^2)^{m/2} \cdot \left( x^{l-m} - \frac{(l-m)(l-m-1)}{2(2l-1)} x^{l-m-2} \pm \dots \right)$$

and obtain by partial integration

$$\begin{aligned} \alpha_{lm}^s &= \frac{2l+1!}{2^{2l+1} l! m!} \int_{-1}^{+1} dx \left( \frac{3}{2} x^2 - \frac{1}{2} \right) (1-x^2)^m \\ &\quad \cdot \left( x^{l-m} - \frac{(l-m)(l-m-1)}{2(2l-1)} x^{l-m-2} \pm \dots \right) \cdot \frac{d^{l+m}}{dx^{l+m}} (x^2 - 1)^l \\ &= (-)^{l+m} \frac{2l+1!}{2^{2l+2} l! m!} \int_{-1}^{+1} (x^2 - 1)^l \cdot \frac{d^{l+m}}{dx^{l+m}} [(1-x^2)^m] \\ &\quad \cdot \left( 3x^2 - 1 \right) \left( x^{l-m} - \frac{(l-m)(l-m-1)}{2(2l-1)} x^{l-m-2} \pm \dots \right) \\ &= (-)^l \cdot \frac{2l+1!}{2^{2l+2} l!} \int_{-1}^{+1} (x^2 - 1)^l \cdot \left[ \frac{3}{2}(l+m+2)(l+m+1)x^2 \right. \\ &\quad \left. - \left( 1 + 3m + 3 \frac{(l-m)(l-m-1)}{2(2l-1)} \right) \right] dx \end{aligned}$$

<sup>1</sup>A. Sommerfeld, Wellenmechanischer Ergänzungsband, p. 63.

$$\begin{aligned}
&= (-)^l \cdot \frac{2l+1!}{2^{2l+2} l!} \int_{-1}^{+1} \left\{ \frac{3}{2} (l+m+2) (l+m+1) (x^2 - 1)^{l+1} \right. \\
&\quad + \left[ \frac{3}{2} (l+m+2) (l+m+1) - \left( 1 + 3m + 3 \frac{(l-m)(l-m-1)}{2(2l-1)} \right) \right] \\
&\quad \cdot (x^2 - 1)^l \Big\} dx \\
&= - \frac{(l+1)!}{(2l+2)(2l+3)} \cdot 3 \cdot (l+m+2) (l+m+1) \\
&\quad + \frac{1}{2} \left( \frac{3}{2} (l+m+2) (l+m+1) - \left( 1 + 3m + 3 \frac{(l-m)(l-m-1)}{2(2l-1)} \right) \right)
\end{aligned}$$

The last form of the expression follows at once from

$$\int_{-1}^{+1} (x^2 - 1)^l dx = (-)^l \cdot \frac{2^{2l} \cdot l!^2}{2l+1!} \cdot 2 \quad (17)$$

By an elementary reduction we obtain finally

$$\alpha_{lm}^1 = \int (P_l^m)^2 P_{l-1}^0 \sqrt{\frac{5}{2}} \sin \vartheta d\vartheta = \frac{l(l+1) - 3m^2}{(2l+3)(2l-1)}$$

In precisely similar fashion one calculates  $\alpha_{lm}^4$ , requiring however the three highest powers in the polynomial:

$$\alpha_{lm}^4 = \frac{3}{4} \cdot \frac{3l^4(l+1)^3 - 30l(l+1)m^2 + 35m^4 - 6l(l+1) + 25m^2}{(2l+5)(2l+3)(2l-1)(2l-3)} \quad (17a)$$

The calculation of the further expansion coefficients now becomes more and more laborious, because more and more terms of the series  $P_l^m(x)$  have to be used; these coefficients are indeed also of little importance for our purposes. For small azimuthal quantum numbers ( $l = 3$  and 4) one can nevertheless easily obtain the next two coefficients  $\alpha_{lm}^3$  and  $\alpha_{lm}^5$ , because the calculation of the coefficients  $\alpha_{lm}^{2l-2}$  and  $\alpha_{lm}^{2l}$  is again simple. To calculate  $\alpha_{lm}^{2l}$  we write the spherical harmonic  $P_{2l}^0$  as a differential expression and  $(P_l^m)^2$  as a polynomial, in which only the highest power of  $x$  is used:

$$\begin{aligned}
(P_l^m)^2 &= \binom{2l}{l-m} \frac{2l+1!}{2^{2l+1} l!} (-)^m (x^{2l} \pm \dots) \\
\sqrt{\frac{2}{4l+1}} P_{2l}^0 &= \frac{1}{2^{2l} \cdot 2l!} \frac{d^{2l}}{dx^{2l}} (x^2 - 1)^{2l}
\end{aligned}$$

By partial integration one finds from

$$\alpha_{lm}^{2l} = \binom{2l}{l-m} \frac{(-)^m (2l+1)}{2^{4l+1} \cdot l!} \cdot \int (x^{2l} \pm \dots) \frac{d^{2l}}{dx^{2l}} (x^2 - 1)^{2l}$$

the result

$$\alpha_{lm}^{2l} = (-)^m \cdot \binom{2l}{l-m} \cdot \frac{\binom{2l}{l}}{\binom{4l+1}{2l}}$$

Similarly one obtains

$$\alpha_{lm}^{2l-2} = (-)^m \cdot \frac{1}{2} \cdot \binom{2l}{l-m} \cdot \frac{\binom{2l-2}{l-1}}{\binom{4l-1}{2l-2}} \cdot \left(1 - \frac{4l-1}{l^2} m^2\right) \quad (17c)$$

TABLE 16

sth-Order Multipole Moments of Electron Density Distributed Proportional to the Square of a Spherical Harmonic ( $P_l^{(1)}$ )<sup>2</sup> = Expansion Coefficient of ( $P_l^{(1)}$ )<sup>2</sup> in Terms of Spherical Harmonics

$$\alpha_{lm}' = \sqrt{\frac{2}{2s+1}} \int_{-1}^{+1} (P_l^{(1)})^2 P_s^0 dx$$

$l =$	1			2			3		
$m =$	0	1	0	1	2	0	1	2	3
$s = 2$	$\frac{2}{5}$	$-\frac{1}{5}$	$\frac{2}{7}$	$\frac{1}{7}$	$-\frac{2}{7}$	$\frac{4}{15}$	$\frac{3}{15} = \frac{1}{5}$	0	$-\frac{5}{15} = -\frac{1}{3}$
$s = 4$	—	—	$\frac{6}{21} = \frac{2}{7}$	$-\frac{4}{21}$	$\frac{1}{21}$	$\frac{6}{33} = \frac{2}{11}$	$-\frac{1}{33}$	$-\frac{7}{33}$	$\frac{3}{33} = \frac{1}{11}$
$s = 6$	—	—	—	—	$-\frac{100}{429}$	$-\frac{75}{429} = -\frac{25}{143}$	$\frac{30}{429} = \frac{10}{143}$	—	$-\frac{5}{429}$

$l =$	4				
$m =$	0	1	2	3	4
$s = 2$	$\frac{20}{77}$	$\frac{17}{77}$	$\frac{8}{77}$	$-\frac{7}{77} = -\frac{1}{11}$	$-\frac{28}{77} = -\frac{4}{11}$
$s = 4$	$\frac{162}{1001}$	$\frac{81}{1001}$	$-\frac{99}{1001} = -\frac{9}{91}$	$-\frac{180}{1001} = -\frac{27}{143}$	$\frac{126}{1001} = \frac{18}{143}$
$s = 6$	$\frac{20}{143}$	$-\frac{1}{143}$	$-\frac{22}{143} = -\frac{2}{13}$	$\frac{17}{143}$	$-\frac{2}{143}$
$s = 8$	$\frac{490}{2431}$	$-\frac{392}{2431}$	$\frac{196}{2431}$	$-\frac{56}{2431}$	$\frac{7}{2431}$

$$\text{Expansion Coefficients } \beta = \int P_l^{(1)} P_l^{(2)} \sin^4 \vartheta \sin \vartheta d\vartheta$$

$l =$	2			3			4		
$m =$	2	2	3	2	3	4	2	1	0
$\mu =$	2	2	1	2	1	0	2	1	0
$\beta =$	$\frac{16}{21}$	$\frac{16}{33}$	$-\frac{16}{165} \sqrt{15}$	$\frac{432}{1001}$	$-\frac{144}{1001} \sqrt{7}$	$\frac{144}{5005} \sqrt{70}$			

We now calculate the constants (16).  $\beta_{lm}$  can be reduced to integrals previously treated:

$$\beta_{lm} = \int (P_l^m)^2 \sin^4 \theta \sin \theta d\theta = \int (P_l^m)^2 \cdot \left( \sqrt{\frac{2}{9}} \cdot \frac{8}{35} \cdot P_4^0 - \sqrt{\frac{8}{5}} \cdot \frac{16}{21} \cdot P_3^0 + \sqrt{2} \cdot \frac{8}{15} \cdot P_2^0 \right)$$

$$\beta_{lm} = 2 \cdot \frac{3l^4(l+1)^2 + 2l(l+1)m^2 + 3m^4 - 14l(l+1) - 15m^2 + 12}{(2l+5)(2l+3)(2l-1)(2l-3)} \quad (18)$$

For the other two cases one obtains by a calculation like the preceding:

$$\beta'_{lm} = -6 \cdot \frac{\sqrt{(l+m+1)(l+m)(l-m+1)(l-m)}}{(2l+5)(2l+3)(2l-1)(2l-3)} \quad (18')$$

$$\beta''_{lm} = 6 \cdot \frac{\sqrt{(l+m+2)(l+m+1)(l+m)(l+m-1)(l-m+2)(l-m+1)(l-m)(l-m-1)}}{(2l+5)(2l+3)(2l-1)(2l-3)} \quad (18'')$$

For  $m = ?$  one has from (18) and (18')

$$\beta_{l0} = 6 \cdot \frac{(l+2)(l+1)l(l-1)}{(2l+5)(2l+3)(2l-1)(2l-3)} \quad (18a)$$

$$\beta'_{l0} = -6 \cdot \frac{\sqrt{(l+3)(l+2)(l-1)(l-2)}}{(2l+5)(2l+3)(2l-1)(2l-3)} \cdot \frac{l(l+1)}{(2l+5)(2l+3)(2l-1)(2l-3)} \quad (18'a)$$

## § 20. The Derivatives of the Lattice Potential

For cubic symmetry none of the three axes is distinguished, so that from

$$\Delta V = 0$$

one has at once

$$\frac{\partial^4 V}{\partial x^4} = \frac{\partial^4 V}{\partial y^4} = \frac{\partial^4 V}{\partial z^4} = 0 \quad (19)$$

The crystal field has no effect on the quadrupole moment of the electron distribution; the fourth-order moment is the first that contributes to the term value. On the other hand, for non-cubic symmetry  $\frac{\partial^2 V}{\partial z^2}$  is of course finite. Accordingly the term splitting is considerable larger [proportional to  $(\frac{\text{orbit radius}}{\text{lattice spacing}})^2$ ] for non-cubic symmetry than for cubic symmetry [proportional to  $(\frac{\text{orbit radius}}{\text{lattice spacing}})^4$ ].

We calculate the  $s$ th derivative of the lattice potential along one axis direction,  $\frac{\partial^s V}{\partial z^s}$ , at the location of a positive ion in a crystal of the NaCl type, using Madelung's method<sup>1</sup>. For this purpose, we use the nucleus of our ion as origin of Cartesian coordinates. The perturbing potential  $V(x, 0, 0)$  consists of a contribution from the row in which the ion itself lies (the X axis), a contribution from the other rows of the plane XY, and a contribution from the other planes  $z = \text{const}$ . We consider the three contributions to  $\frac{1}{s!} \frac{\partial^s V}{\partial x^s}$  individually, writing  $a$  for the distance between nearest neighbors and  $E$  for the ionic charge.

### 1. Contribution to the potential from ions of the row in question:

$$\begin{aligned} V_1(x, 0, 0) &= -\frac{E}{a} \left( \frac{1}{1 - \frac{x}{a}} + \frac{1}{3 - \frac{x}{a}} + \dots + \frac{1}{1 + \frac{x}{a}} + \frac{1}{3 + \frac{x}{a}} + \dots \right) \\ &\quad + \frac{E}{a} \left( \frac{1}{2 - \frac{x}{a}} + \frac{1}{4 - \frac{x}{a}} + \dots + \frac{1}{2 + \frac{x}{a}} + \frac{1}{4 + \frac{x}{a}} + \dots \right) \end{aligned}$$

Accordingly,

$$\frac{1}{s!} \left( \frac{\partial^s V_1}{\partial x^s} \right)_{x=0} = 0$$

when  $s$  is odd. For even  $s$  one has

$$\begin{aligned} \frac{1}{s!} \left( \frac{\partial^s V_1}{\partial x^s} \right)_s &= -\frac{2E}{a^{s+1}} (1^{-(s+1)} - 2^{-(s+1)} + 3^{-(s+1)} \pm \dots) \\ &= -\frac{2E}{a^{s+1}} r_{s+1} \end{aligned} \tag{20a}$$

The values are

$$r_3 = 0.9016, r_5 = 0.9722, r_7 = 0.9926, \text{ etc}$$

2. Contribution of neighboring rows. The  $\rho$ th neighboring row at the distance  $y = \rho a$  contains a positive or negative ion at the point  $(0, \rho a, 0)$ , depending on whether  $\rho$  is even or odd, and produces on the x axis the potential<sup>2</sup>

$$\begin{aligned} V_\rho(x, 0, 0) &= \frac{4E}{a} (-)^{\rho} \sum_{l=1, 3, 5, \dots} K_0(\pi l \rho) \cos \frac{\pi l x}{a} \\ \frac{1}{s!} \frac{\partial^s V_\rho}{\partial x^s} &= \frac{4E}{a^{s+1}} (-)^{\rho + \frac{s}{2}} \frac{\pi^s}{s!} \sum_{l=1, 3, 5, \dots} K_0(\pi l \rho) l^s \cos \frac{\pi l x}{a} \end{aligned}$$

for even  $s$ . We sum over all rows of the XY plane (each appears twice, to "right" and "left" of the row containing our ion) and set  $x = 0$ :

<sup>1</sup> $K_0(x) = H_0^{(1)}(ix)$  = Hankel function of first type with imaginary argument.  
<sup>2</sup>E. Madelung, Physikal. Ztschr. Vol. 19, p. 524 (1918).

$$\frac{1}{s!} \left( \frac{\partial^s V_0}{\partial x^s} \right)_0 = \frac{8E}{a^{s+1}} \cdot (-)^{\frac{s}{2}} \frac{\pi^s}{s!} \sum_{l=1,3,5,\dots} b_l \sum_{\rho=1,2,3,\dots} (-)^{\rho} K_0(\pi l \rho) \quad (20b)$$

3. Contribution of the neighboring plane at distance  $z = \rho a$  (at the point  $(0, 0, \rho a)$ ) there is an ion with the charge  $(-)^{\rho} E$ :

$$V'_e = (-)^e \frac{8E}{a} \sum_{l=1,3,5,\dots} \sum_{m=1,3,5,\dots} \frac{e^{-\pi e \sqrt{l^2+m^2}}}{\sqrt{l^2+m^2}} \cos \frac{\pi l x}{a}$$

$$\frac{1}{s!} \frac{\partial^s V'_e}{\partial x^s} = \frac{8E}{a^{s+1}} (-)^{\frac{s}{2}} \frac{\pi^s}{s!} \sum_{l=1,3,5,\dots} \sum_{m=1,3,5,\dots} \frac{e^{-\pi e \sqrt{l^2+m^2}}}{\sqrt{l^2+m^2}} b_l$$

$$(-)^e \cos \frac{\pi l x}{a} \quad (\text{for even } s)$$

Contribution of all neighboring planes:

$$\frac{1}{s!} \left( \frac{\partial^s V_0}{\partial x^s} \right)_0 = \frac{16E}{a^{s+1}} (-)^{\frac{s}{2}} \frac{\pi^s}{s!} \sum_{l=1,3,5,\dots} \sum_{m=1,3,5,\dots} (-)^{\rho} \frac{e^{-\pi e \sqrt{l^2+m^2}}}{\sqrt{l^2+m^2}} \quad (20c)$$

Thus the total value of the  $s$ th derivative of the perturbing potential at the lattice point is

$$\frac{1}{s!} \left( \frac{\partial^s V}{\partial x^s} \right)_0 = - \frac{2E}{a^{s+1}} r_{s+1} + \frac{8E}{a^{s+1}} (-)^{\frac{s}{2}} \frac{\pi^s}{s!} \sum_{l=1,3,5,\dots} b_l \beta_l \quad (20)$$

where

$$\beta_l = \sum_{\rho=1,2,3,\dots} (-)^{\rho} \left( K_0(\pi l \rho) + 2 \sum_{m=1,3,5,\dots} \frac{e^{-\pi e \sqrt{l^2+m^2}}}{\sqrt{l^2+m^2}} \right) \quad (20d)$$

$$\begin{aligned} \beta_1 &= -0.0450 & \beta_3 &= -0.850 \cdot 10^{-4} \\ \beta_5 &= -0.92 \cdot 10^{-7} & \beta_7 &= -0.138 \cdot 10^{-9} \end{aligned}$$

Then we have, for example

$$\frac{1}{4!} \left( \frac{\partial^4 V}{\partial x^4} \right)_0 = -3.58 \frac{E}{a^4} \quad (20e)$$

$$\frac{1}{6!} \left( \frac{\partial^6 V}{\partial x^6} \right)_0 = -0.82 \frac{E}{a^6}$$

Now we suppose that our NaCl crystal is stretched somewhat in the direction of one cube edge Z, so that we get a crystal of tetragonal symmetry<sup>1</sup>. Let the ratio of the four-fold axes to the two-fold axes be  $\frac{c}{a} = 1 + \epsilon$ . Then the second derivatives of the perturbing potential along the directions of the axes of course no longer vanish. The contribution of the ions in the XY plane to  $\frac{\partial^2 V}{\partial x^2}$  indeed remains constant, but the contribution of the parallel planes  $z = pa(1 + \epsilon)$  becomes smaller, as is at once obvious physically and comes about formally through the fact that the exponent of every exponential function in Eq. (20c) acquires the factor  $\frac{c}{a} = 1 + \epsilon$ . Since, now, the parallel planes make a positive contribution<sup>2</sup> to  $\frac{\partial^2 V}{\partial x^2}$  we have

$$\frac{\partial^2 V}{\partial x^2} = \frac{\partial^2 V}{\partial y^2} < 0 \quad \text{for } \epsilon > 0$$

and thus because  $\Delta V = 0$ , accordingly

$$\frac{\partial^2 V}{\partial z^2} > 0$$

This means: In a sufficiently stretched NaCl crystal those terms lie lowest for which the second-order moment of the electron density in the direction of the tetragonal axis is positive (cf. Eq. (14)), thus the terms of smallest electric quantum number m (upper index of the spherical harmonic  $P_m^m$ ). Here the assumption is that the stretching is large enough so that the effect of the fourth-order moment is negligible in comparison with that of the second-order moment (§ 22). For a shortened crystal of the NaCl type, the situation is of course the opposite, and also the sign is reversed for the electrons of a negative ion.

### § 21. The Splitting Pattern for Cubic Symmetry

The magnitude of the term splitting for cubic symmetry is mainly determined by the potential energy of the fourth-order multipole moments of the electron density in the crystal field. According to § 18, the position of the term  $(n, l, \lambda)$  in relation to the center of gravity of all terms with the same  $n$  and  $l$  is given by

$$E_l = -e \overline{r^4} \frac{\partial^4 V}{\partial z^4} \int P_{ll}^l \left( P_4^0 + \frac{5}{8} \sin^4 \vartheta \cos 4\varphi \right) \sin \vartheta d\vartheta d\varphi \quad (21)$$

<sup>1</sup> Such a crystal is not found in nature, but it would be the simplest possible structure of a tetragonal ionic crystal.

<sup>2</sup> For  $(-)^{3/2} = -1$ , and the main contribution is made by the first parallel plane on each side ( $\rho = 1$ ); on account of the factor  $(-)^p$ ,  $\frac{\partial^2 V}{\partial x^2}$  is thus positive.

where  $P_{l\lambda}$  is any one of the angle-dependent eigenfunctions that belong to the term  $(n, l, \lambda)$ , accordingly a linear combination of spherical harmonics of  $l$ th order.<sup>1</sup> The absolute value of the splitting in a crystal of the NaCl type with monovalent ions is given, according to Eq. (20e), apart from a factor of order of magnitude 1, by

$$\begin{aligned} D &= -e \frac{\overline{r^4}}{4!} \frac{\partial^4 V}{\partial z^4} = \frac{e^4}{a^4} \overline{r^4} \cdot 3.58 \approx \frac{e^4}{5a_H} \cdot \frac{3.58}{5^4} \\ &= 1.1 \cdot 10^{-3} \cdot \frac{e^4}{a_H} = 2.1 \cdot 10^{-3} \cdot \text{Rydberg const.} \approx 250 \text{ cm}^{-1} \end{aligned}$$

if it is assumed that the radius of the electron orbit is equal to the hydrogen radius  $a_H$  and the lattice spacing is  $a = 5a_H$ . Accordingly the splitting is of the order of magnitude of the multiplet separation. Consequently our calculation of the terms is not exact, since it not only neglects the interaction between spin and orbit, although this is of the same order of magnitude as the effect of the crystalline field, but even the interaction of the individual electrons outside closed shells. Nevertheless we shall carry the calculation further as an illustration of the group-theoretical determination of the splitting.

If we now consider, for example, a positive ion in a crystal of the NaCl type, the relative position of the terms is given, apart from a positive factor  $D$  that is a constant for all terms of the same  $n$  and  $l$ , by

$$e_l = \int P_{l1}^* \left( P_4^0 + \frac{5}{8} \sin^4 \vartheta \cos 4\varphi \right) \sin \vartheta d\vartheta d\varphi \quad (21a)$$

For a d electron, for example, the position of the two-fold degenerate crystal term  $d_y$  relative to the center of gravity of the two terms  $d_y$  and  $d_z$  is given by

$$E_y - E_0 = \frac{2}{7} D$$

<sup>1</sup>The contribution of the neglected terms of 6th order would be of a size, relative to the terms of 4th order, of say

$$\frac{\frac{\overline{r^6}}{6!} \frac{\partial^6 V}{\partial z^6}}{\frac{\overline{r^4}}{4!} \frac{\partial^4 V}{\partial z^4}} = \frac{0.92 \frac{E}{a^4}}{3.58 \frac{E}{a^4}} \frac{\overline{r^6}}{\overline{r^4}} \approx \frac{1}{4} \left( \frac{\text{orbit radius}}{\text{lattice spacing}} \right)^2 \approx 0.01$$

i.e., on the basis of data for the NaCl type of crystal, the neglect causes only say 1 percent error.

for the eigenfunction  $d_\gamma$  belongs to  $P_2^0$ , and according to Table 16 one has  $\int (P_2^0)^2 P_4^0 dx = 2/7$ . One of the eigenfunctions for the three-fold term  $d_\epsilon$  is  $P_2^1 e^{i\varphi}$ , and since, according to Table 16,  $\int P_2^1 e^{i\varphi} P_2^1 e^{-i\varphi} P_4^0 dx = 4/21$ , we have<sup>1</sup>

$$E_\epsilon - E_0 = - \frac{4}{21} D$$

For a positive ion in a crystal of the NaCl type the two-fold term, for which the maximum electron density is concentrated along the four-fold axes (§ 14), accordingly lies higher than the three-fold term with its electron concentration along the three-fold axes. This is very reasonable: The nearest negative neighbors of the ion lie on the four-fold axes and naturally try to repel the electrons of the positive ion as far from themselves as possible. For a negative ion, the relationships are of course reversed, and they would also reverse on going over to the CsCl type.

An electron in the f state can have its maximum probability of occurrence either on the body diagonals (single term  $f_B$ ), along the cube edges (three-fold term  $f_\delta$ ), or along the face diagonals (three-fold term  $f_\epsilon$ ). One of the eigenfunctions belonging to the term  $f_\delta$  is  $P_3^0$ , so that

$$E_\delta - E_0 = + \frac{2}{11} D$$

The term  $f_B$  has the eigenfunction  $\sqrt{2} P_3^2 \sin 2\varphi$ , and one of those belonging to  $f_\epsilon$  is  $\sqrt{2} P_3^2 \cos 2\varphi$ , so that

$$E_\delta + E_\epsilon - 2E_0 = 2 \int (P_3^2)^2 V \psi_{n1}^2(r) d\tau = - 2 \cdot \frac{7}{33} D$$

Making use of the definition of the center of gravity of the terms,

$$7E_0 = E_\delta + 8E_\epsilon + 9E_\epsilon$$

one gets for the positions of the terms

---

<sup>1</sup>As also follows from the definition of the center of gravity of the terms, the relation  $2E_\gamma + 3E_\epsilon = 5E_0$ .

$$E_g - E_0 = -\frac{4}{11} D$$

$$E_t - E_0 = -\frac{2}{33} D$$

$$E_\epsilon - E_0 = +\frac{2}{11} D$$

For the positive ion of the NaCl crystal the term  $f_g$  lies lowest, because here the electron has its density maximum on the body diagonals, farthest removed from the negative neighbor ions; the term  $f_\delta$  lies highest (density maximum along the edges); and  $f_\epsilon$ , with the maximum along the face diagonals, takes an intermediate position. The ratio of the separations of the terms is

$$(E_g - E_0):(E_t - E_0) = 4:5$$

and indeed this holds always for cubic symmetry, not only for the NaCl type of crystal.

Finally we come to the splitting of the  $g$  term, and find, using Table 16:

$$E_a - E_0 = 14 \cdot \frac{18}{1001} D$$

$$E_g - E_0 = 7 \cdot \frac{18}{1001} D$$

$$E_\epsilon - E_0 = 2 \cdot \frac{18}{1001} D$$

$$E_t - E_0 = -13 \cdot \frac{18}{1001} D$$

$g_a$  corresponds to a density maximum on the four-fold axes,  $g_\epsilon$  to one on the three-fold axes.

#### § 22. The Splitting Pattern for Tetragonal Symmetry. Measure of the "Tetragonality"

The position of a term with the quantum numbers ( $n, l, \lambda$ ) relative to the center of gravity of all the terms with the same  $n$  and  $l$  is

$$E_\lambda - E_0 = -e \frac{\overline{r^3}}{2!} \left( \frac{\partial^3 V}{\partial z^3} \right)_0 \alpha_{l1} - e \frac{\overline{r^4}}{4!} \cdot \left( \frac{\partial^4 V}{\partial z^4} \cdot \alpha'_{l1} + \frac{1}{8} \left( 8 \frac{\partial^4 V}{\partial z^4} - 3 \frac{\partial^2 V}{\partial z^2} \right) \beta_{l1} \right) \quad (22)$$

where (cf. § 18)

$$\begin{aligned}\alpha_{11} &= \int P_{11}^1 P_4^0 d\tau \quad \alpha'_{11} = \int P_{11}^1 P_4^0 d\tau \\ \beta_{11} &= 2 \int P_{11}^1 \sin^4 \vartheta \cos 4\varphi d\tau\end{aligned}\tag{22a}$$

Here the assumption is used that the representation  $\gamma_\lambda$  of the tetragonal group has belonging to it only the one term  $E_\lambda$  with the eigenfunction  $P_{1\lambda}$ . If one goes over from tetragonal symmetry to cubic symmetry, then  $\frac{\partial^2 V}{\partial z^2}$  vanishes, while  $\frac{\partial^4 V}{\partial z^4}$  and  $\frac{\partial^4 V}{\partial x^4}$  change only relatively little. As long as these fourth-order terms play any part at all, i.e., for nearly cubic symmetry, we can also set  $\frac{\partial^4 V}{\partial x^4} = \frac{\partial^4 V}{\partial z^4}$ . It now seems suitable to relate the term displacement to the quantity

$$D = -e \frac{\vec{r}^3}{4!} \frac{\partial^4 V}{\partial x^4}$$

in order to make possible a comparison with the relationships for cubic symmetry:

$$E_4 - E_0 = D \left( \epsilon_4 + \frac{\vec{r}^3}{r^3} \cdot \frac{\frac{1}{2!} \left( \frac{\partial^4 V}{\partial z^4} \right)_0}{\frac{1}{4!} \left( \frac{\partial^4 V}{\partial x^4} \right)_0} \alpha_{11} \right)\tag{23}$$

with

$$\epsilon_4 = \alpha'_{11} + \frac{5}{16} \beta_{11} = \int P_{11}^1 \left( P_4^0 + \frac{5}{8} \sin^4 \vartheta \cos 4\varphi \right) d\tau\tag{21a}$$

Here the constant  $D$  has only a slight dependence on whether the atom has cubic or tetragonal symmetry. For the NaCl type  $D = 3.58 e^2/a^6$ . We are primarily interested in the second quantity in the parentheses, which vanishes for cubic symmetry and for tetragonal symmetry represents the difference from the cubic case. We call it the effective tetragonality. Setting

$$u = \frac{\vec{r}^3}{r^3} \cdot \frac{\frac{1}{2!} \left( \frac{\partial^4 V}{\partial z^4} \right)_0}{\frac{1}{4!} \left( \frac{\partial^4 V}{\partial x^4} \right)_0}$$

we have

$$E_1 - E_0 = D(s_1 + u \alpha_{11})$$

The "effective tetragonality" determines the relative position of the Stark-effect components of an electron term for tetragonal symmetry. It is inversely proportional to the square of the "orbit radius" of the electron. In order to obtain a constant for the symmetry of the atom, we define the absolute tetragonality

$$U = \frac{\frac{1}{2!} \left( \frac{\partial^4 V}{\partial x^4} \right)_0}{\frac{1}{4!} \left( \frac{\partial^4 V}{\partial z^4} \right)_0}$$

as the ratio of the second to the fourth derivative of the perturbing lattice potential with respect to the direction of the tetragonal axis, at the position of the nucleus of the atom. For cubic symmetry  $U = 0$ , and we shall call a symmetry nearly cubic when the tetragonality  $U$  is small (say, smaller than 0.1); on the other hand, for large  $U$  we have to do with decidedly tetragonal symmetry<sup>1</sup>. The introduction of the tetragonality is justified by the fact that it is a criterion for the relative positions of the terms, and thus also for the most stable electron distribution in an atom in a prescribed position in the crystal.

To be sure, we have confirmed this significance of the tetragonality so far only for the case in which only one term belongs to each irreducible representation of the tetragonal group. We shall base our proof that it has the same significance (on the same hypothesis  $\frac{\partial^4 V}{\partial x^4} \approx \frac{\partial^4 V}{\partial z^4}$ ) also in the case of several terms with the same representation on the example already begun in § 11 (this can easily be generalized). The two terms that belong to the two-dimensional representation for the azimuthal quantum number  $l = 3$  are given by

$$E_b', E_b'' = \frac{e_{11} + e_{33}}{2} \pm \sqrt{\left(\frac{e_{11} - e_{33}}{2}\right)^2 + e_{13}^2} \quad (6)$$

<sup>1</sup> For a stretched-out crystal of the NaCl type, the tetragonality is always negative (cf. § 20), and for small stretchings

$$U \approx -1.71 \epsilon$$

and corresponding to this, for an orbit radius of, say,  $1/4$  of the lattice spacing, the effective tetragonality is

$$U \approx -30 \epsilon = -30 \frac{a}{c-a}$$

For a shortened crystal axis, the sign is reversed; on the other hand it is independent of the sign of the charge of the ion considered.

Here, according to Eq. (5), and by the use of Eqs. (14) and (15) and Table 16, we have

$$\begin{aligned}\epsilon_{11} &= -eV_0 - \frac{1}{5}e \frac{\overline{r^4}}{2!} \left( \frac{\partial^4 V}{\partial x^4} \right)_0 - \frac{1}{33}e \frac{\overline{r^4}}{4!} \left( \frac{\partial^4 V}{\partial z^4} \right)_0 \\ \epsilon_{33} &= -eV_0 + \frac{1}{3}e \frac{\overline{r^4}}{2!} \left( \frac{\partial^4 V}{\partial x^2} \right)_0 - \frac{1}{11}e \frac{\overline{r^4}}{4!} \left( \frac{\partial^4 V}{\partial z^2} \right)_0 \\ \epsilon_{13} &= \frac{16}{185} \sqrt{15} e \frac{\overline{r^4}}{4!} \cdot \frac{1}{16} \left( 8 \frac{\partial^4 V}{\partial x^4} - 3 \frac{\partial^4 V}{\partial z^4} \right)_0 \approx \frac{\sqrt{15}}{33} \frac{\overline{r^4}}{4!} \left( \frac{\partial^4 V}{\partial x^4} \right)_0\end{aligned}$$

Then

$$\begin{aligned}\frac{\epsilon_{11} + \epsilon_{33}}{2} + eV_0 &= D \left( \frac{2}{33} - \frac{u}{15} \right) \\ \frac{\epsilon_{11} - \epsilon_{33}}{2} &= D \left( -\frac{1}{33} + \frac{4u}{15} \right) \\ \epsilon_{13} &= -D \cdot \frac{\sqrt{15}}{33}\end{aligned}$$

$$\begin{aligned}E_s' - E_0 &= D \left( \frac{2}{33} - \frac{u}{15} + \frac{4}{3} \sqrt{\frac{u^2}{5^2} - \frac{u}{110} + \frac{1}{11^2}} \right) \\ E_s'' - E_0 &= D \left( \frac{2}{33} - \frac{u}{15} - \frac{4}{3} \sqrt{\frac{u^2}{5^2} - \frac{u}{110} + \frac{1}{11^2}} \right)\end{aligned}\tag{25}$$

Here also the position of the terms turns out to depend mainly on the effective tetragonality  $u$ ; the proportionality factor  $D$  is the same as in Eq. (23a).

For small effective tetragonality (almost cubic symmetry) one has by Eq. (25)

$$\begin{aligned}E_s' - E_0 &= D \left( \frac{2}{11} - \frac{2u}{15} + \frac{11}{40} u^2 + \dots \right) \\ E_s'' - E_0 &= D \left( -\frac{2}{33} - \frac{11}{40} u^2 + \dots \right)\end{aligned}\tag{25a}$$

That is: For cubic symmetry ( $u = 0$ ),  $E_s'$  goes over into the term  $f_g$ , and  $E_s''$  into the term  $f_\epsilon$ . For a slight departure from cubic symmetry, the term value varies continuously with the departure. For pronounced tetragonal symmetry ( $u \gg l$ ), on the other hand,

$$E_s' - E_0 = D \left( -\frac{u}{15} + \frac{2}{33} + \frac{4}{15} |u| - \frac{1}{33} \frac{u}{|u|} + \frac{1}{u} (\dots) \right)$$

(The positive sign of the square root belongs to  $E_5'$ , so that  $u$  must be inclosed in absolute value marks). For large positive  $u$  one gets

$$E_5' - E_0 = D \left( -\frac{u}{3} + \frac{1}{33} + \frac{1}{u} \dots \right) \quad (25b)$$

and on the other hand for  $u < 0$ ,

$$E_5' - E_0 = D \left( -\frac{u}{3} + \frac{1}{11} + \frac{1}{u} \dots \right) \quad (25c)$$

Similarly,

$$\begin{aligned} E_5'' - E_0 &= D \left( -\frac{u}{3} + \frac{1}{11} + \frac{1}{u} \dots \right) \quad u > 0 \\ E_5'' - E_0 &= D \left( -\frac{u}{5} + \frac{1}{33} + \frac{1}{u} \dots \right) \quad u < 0 \end{aligned} \quad (25d)$$

That is: For pronounced tetragonal symmetry it is unimportant that  $E_5'$  and  $E_5''$  are two terms with the same representation of the tetragonal group. One gets two terms which (apart from slight corrections of the 6th order) simply correspond to the two orientations of the electron's angular momentum  $l = 3$  with the components  $m = 1$  and  $m = 3$  in the direction of the tetragonal axis:

$$E_5' - E_0 = e_{33} - E_0 = D \left( -\frac{u}{3} + \frac{1}{11} \right) = -\frac{e}{3} \cdot \frac{\bar{r}^3}{2!} \left( \frac{\partial^3 V}{\partial r^3} \right)_0 - \frac{e}{11} \frac{\bar{r}^4}{4!} \left( \frac{\partial^4 V}{\partial r^4} \right)_0$$

$$E_5'' - E_0 = e_{11} - E_0 = D \left( -\frac{u}{5} + \frac{1}{33} \right) = -\frac{e}{5} \cdot \frac{\bar{r}^3}{2!} \left( \frac{\partial^3 V}{\partial r^3} \right)_0 - \frac{e}{33} \frac{\bar{r}^4}{4!} \left( \frac{\partial^4 V}{\partial r^4} \right)_0$$

But for positive tetragonality  $E_5'$  corresponds to an orientation of the angular momentum with the component  $m = 1$  in the direction of the tetragonal axis, whereas for negative  $u$  it corresponds to the orientation with  $m = 3$ . Independently of the value of  $u$ ,  $E_5'$  always remains the higher of the two terms, and one cannot consistently assign to it the same electric quantum number, say  $m = 3$ , for all  $u$ , because this in one case corresponds to the lower and in the other to the higher term. If, beginning with positive tetragonality, we think of the crystal as being adiabatically deformed and approaching cubic symmetry, then it no longer has any meaning to speak

of a component  $m = 1$  in the direction of the tetragonal axis, as soon as this tetragonal axis is no longer sufficiently distinguished from the other two axes. Only when the deformation has proceeded so far beyond the cubic case that the symmetry has again become pronouncedly, but now negatively, tetragonal, can we again define a component of the angular momentum of the electron orbit in the direction of the tetragonal axis, but this is now  $m = 3$ . This example can be regarded as an illustration of the general theorem that terms of the same representation never cross over each other. We could, of course, also write the zeroth-order eigenfunctions (eq. (7), § 11) in terms of  $u$ , and would obtain the same transition from  $P_3^1$  through the eigenfunction for cubic symmetry and on to  $P_3^3$ , when we let  $u$  go from large positive values through zero to large negative values.

The dependence of the term values, calculated relative to the center of gravity of the terms, on the effective tetragonality  $u$  is shown in Figs. 6-8; the term values are plotted in terms of the factor<sup>1</sup>  $D = -e \frac{r^4}{4!} \frac{\partial^4 V}{\partial z^4}$ . For added clarity abscissas are given in terms not only of the effective tetragonality  $u$  but also of the ratio of axes  $c/a$  which would correspond to the tetragonality  $u$  for a stretched crystal of the NaCl type if the radius of the electron orbit is taken to be about  $1/4$  of the lattice spacing.

Fig. 6 shows the splitting pattern of the d term as function of the tetragonality. Since no representation has two terms corresponding to it, every term can have assigned to it an  $m$ -value (electric quantum number, component of angular momentum in the direction of the tetragonal axis) and an angular eigenfunction independent of  $u$ , and in addition each term value depends linearly on  $u$ . For pronounced tetragonal symmetry one gets a wide splitting proportional to  $\left(\frac{\text{orbit radius}}{\text{lattice spacing}}\right)^2$  between terms with different values of  $m$ , for which the usual interval rule (separation between  $m$  and  $m + 1$  proportional to  $(m + 1)^2 - m^2 = 2m + 1$ ) holds approximately, and a narrow splitting proportional to  $\left(\frac{\text{orbit radius}}{\text{lattice spacing}}\right)^4$  between the two terms with the eigenfunctions

$$\sqrt{2} P_3^1 \cos 2\varphi \quad \text{and} \quad \sqrt{2} P_3^1 \sin 2\varphi$$

<sup>1</sup>In reality this factor itself will of course change, though indeed slowly, with the change of the tetragonality, but this change will depend on the special structure of the crystal, while the relative positions and separations of the terms depend only on the value of the tetragonality.

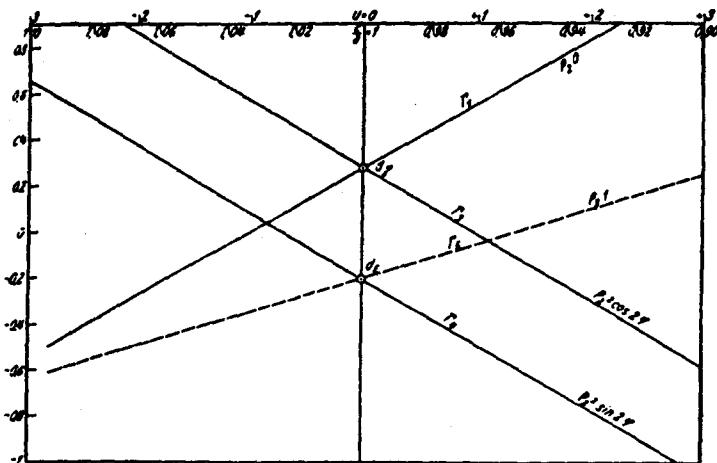


Fig. 6. Splitting pattern of the d term for tetragonal symmetry.

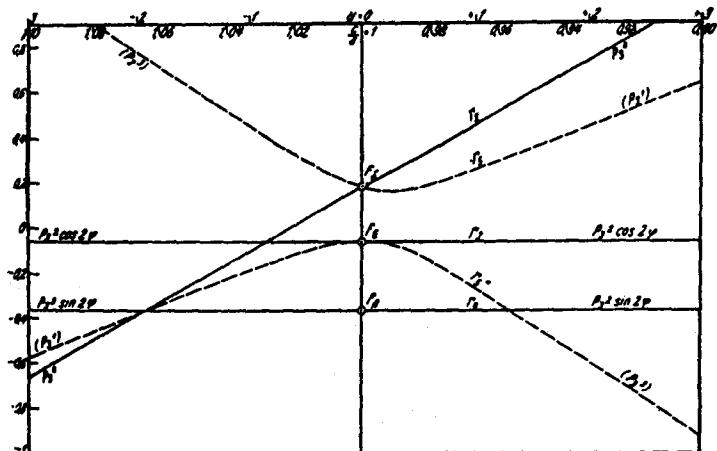


Fig. 7. Splitting pattern of the f term for tetragonal symmetry.

----- two-fold degenerate terms  
— simple terms

Fig. 7 shows the splitting pattern of the f term as a function of u. The curves for the terms  $E_1^f$  and  $E_3^f$  form a hyperbola whose asymptotes are the straight lines  $\epsilon_{11} - \epsilon_0$  and  $\epsilon_{33} - \epsilon_0$ . These lines would represent the terms belonging to the electric quantum numbers 1 and 3, if these quantum numbers could be defined for all u.

Fig. 8 shows the splitting pattern of the g term, in which four terms are represented as functions of u by hyperbolas. For large tetragonality, one again gets an ordering of the terms according to m; the term  $m = 2$  is split up once again (eigenfunctions  $\sqrt{2} P_4^2 \cos 2\varphi$  and  $\sqrt{2} P_4^2 \sin 2\varphi$ ), but the corresponding splitting

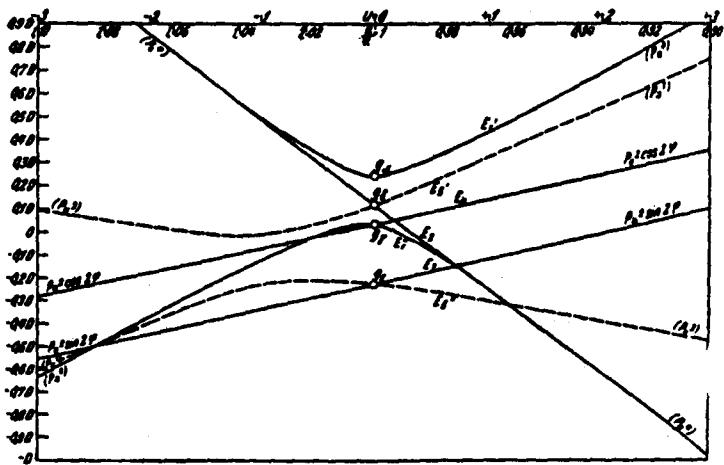


Fig. 8. Splitting pattern of the g term for tetragonal symmetry.

for  $m = 4$  practically vanishes, because it is produced in lowest order by the multipole moment of 8th order.

As regards the absolute magnitude of the splitting, for pronounced tetragonal symmetry, this can reach considerably larger values than for cubic symmetry. If we take, say, a crystal of the shortened NaCl type, then for an axis ratio

$$\frac{c}{a} = \frac{7}{8}$$

one has, say,

$$\frac{1}{2\Gamma} \left( \frac{\delta^2 V}{\delta x^2} \right)_0 = -1 \cdot \frac{E}{a^2}$$

and thus for an orbit radius of  $1/5$  the lattice spacing, and for singly charged ions, the term value is

$$E_1 - E_0 \approx + \frac{r^2}{a^3} \cdot \frac{e^2}{a} \cdot \alpha_{11} \approx \frac{1}{25} \frac{e^2}{a} \alpha_{11} \approx \\ 0.008 \cdot 2 \cdot \text{Rydberg constant} \cdot \alpha_{11} \approx 2000 \text{ cm}^{-1}$$

Thus the splitting can easily exceed  $1000 \text{ cm}^{-1}$ .

Since the tetragonality controls the relative position of the crystal terms, it determines the most stable arrangement of electrons in the crystal, as has been said before. For example, in the case of strong negative tetragonality, for a d electron of a positive ion the orientation of the electron along the tetragonal axis is the most stable (eigenfunction  $P_2^0$ ); for less pronounced stretching one finds

an energy minimum for an oblique orientation, in which the maximum of the density is located on a cone around the tetragonal axis with aperture angle  $\pi/2$  ( $P_2^1$ ). For cubic symmetry the stablest state has the density maximum along the three-fold axes, and finally for positive tetragonality (shortened NaCl crystal) it goes over onto the face diagonals of the plane perpendicular to the tetragonal axis (eigenfunction  $\sqrt{2} P_2^2 \sin 2\phi$ ). Similar considerations can be carried through by means of Figs. 6-8 for negative ions and for other electronic terms. The relative term separations shown in the diagrams are independent of the special structure of the crystal, as is indeed the whole concept of the tetragonality.

### § 23. Prospects for Applications of the Theory

This theory gives a survey of the effects of electric fields of definite symmetries on an atom. Accordingly it will be possible to apply it to advantage in the treatment of symmetrical molecules<sup>1</sup>. A direct physical confirmation should be obtainable by analyses of the spectra of crystals; it appears that the salts of the rare earths, which are the only ones giving sharp absorption lines, can serve as verification for the theory<sup>2</sup>. Furthermore it would be conceivable that when supplemented by a theory of the exchange effects this theory could provide an explanation of polymorphic transitions, but we leave this question to one side for the present. Some importance attaches to the negative result that for cubic symmetry P terms do not split up (and more generally S terms do not). Finally, it is possible to get a survey of the departures of the atomic symmetry in a crystal from spherical symmetry; a comparison of the value of the term splitting of an electron with quantum numbers ( $n, l$ ) with its term value in the free atom also provides a quantitative estimate of this departure. For tetravalent carbon (diamond) one should, to be sure, expect no important departure from spherical symmetry in zeroth approximation, since the ground term is a  $^4S$  term, so that only the spin can take different orientations, and not the orbital angular momentum. Presumably in this case, it is the deformation of the L shell that will cause the departure from spherical symmetry that is observed by means of x-rays.

(Received July 20, 1929)

<sup>1</sup>See the remarks in § 12, 13, etc. regarding the relations of the present study to that made by Ehler for  $\text{CH}_4$  loc. cit.

<sup>2</sup>I owe my thanks to Dr. Schutz (Tübingen) for pointing this out.

Note added in proof: The absorption lines in question show a splitting in a magnetic field into only a few (often 2) components, which are often widely separated. If one recalls that the crystalline field produces a considerable splitting-up of the terms, this is easily understandable: The unperturbed crystal terms (without magnetic field) are in general only two-fold degenerate or not degenerate at all, and the magnetic field removes this last remaining directional degeneracy and splits the term into only one or two components. On the other hand the separation of these components is proportional to the magnetic quantum number  $m$ , which can take very sizable values because of the large total angular momenta ( $j$  up to say 10) of the rare earths. A more thorough analysis of these relations is not possible at present on account of the unspicuous condition of the experimental information.

**The Electron Affinity of Hydrogen**  
*Zeits. Physik* **57**, 815 (1929)

The negative hydrogen ion,  $H^-$ , is stable. To my knowledge, this paper is the first calculation of its binding energy. The ion is important in the outer part of the sun and similar stars where it provides a substantial fraction of the opacity.

# The Electron Affinity of Hydrogen

*Zeits. Physik* **57**, 815.

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The old quantum theory was unable to calculate the binding energy of a second electron to the hydrogen atom; in fact, two authors concluded that a negative hydrogen ion could not exist at all.

I use the variational method pioneered by Hylleraas<sup>1</sup>. I choose the trial function

$$\psi = e^{-ks/2} (1 + \alpha k u + \beta k^2 t^2) , \quad (1)$$

where  $k$ ,  $\alpha$  and  $\beta$  are parameters which are varied so as to make the energy a minimum, and

$$s = r_1 + r_2 , \quad t = r_1 - r_2 , \quad u = r_{12} . \quad (2)$$

Here  $r_1$  and  $r_2$  are the distances of the two electrons from the proton and  $r_{12}$  their distance from each other. All distances are measured in units of the Bohr radius

$$a_0 = \hbar^2 / me^2 = 0.528 \times 10^{-8} \text{ cm} . \quad (3)$$

Variation of the parameters gives the result

$$\begin{aligned} k &= 1.535 , \quad \alpha = 0.20 , \quad \beta = 0.05 \\ E &= -1.0506 \text{ Ry} \end{aligned} \quad (4)$$

---

<sup>1</sup>E. A. Hylleraas, *Z. Phys.* **54**, 347, 1929.

where  $Ry$  is the binding energy of the  $H$  atom,

$$Ry = e^2/2a_0 = 13.6 \text{ eV} . \quad (5)$$

Comparing the calculation with that of the  $He$  ground state by Hylleraas, I estimate the likely improvement of the energy value by further approximations, and thus find the binding energy of the extra electron,

$$\varepsilon = 0.0537 \pm 0.0003 Ry = 0.73 \text{ eV} . \quad (6)$$

The density distribution of the electrons according to the wave function (1) is calculated: It is found to extend considerably further than one would find with the simplest trial function

$$\psi = e^{-ks/2} , \quad (7)$$

with  $k = 1.6875$ .

It is shown that there are probably no discrete excited states of the  $H^-$  ion.

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## **Theory of the Passage of Fast Corpuscular Rays Through Matter**

*Ann. Physik* **5** (5), 325–400 (1930)

After Max Born published the theory of atomic collisions, I was able to simplify it considerably, and to calculate cross sections for elastic and inelastic collisions, and for ionization. I was able to find sum rules, especially for the rate of energy loss of a charged particle going through matter. This is closely related to the rate of ionization which can be measured and is widely used in nuclear and particle physics experiments. Together with a measurement of the momentum, by the deflection in a magnetic field, it permits the calculation of the mass of the particle. The results of this paper have also been used to calculate the relation between range and energy of particles. The theory has been generalized to include the effects of special relativity (*Zeits. Physik* **76**, 293, 1932). An up-to-date review has been published by J. Lindhard and A. H. Sorensen (1995).

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THEORY OF THE PASSAGE  
OF FAST CORPUSCULAR RAYS THROUGH MATTER

TRANSLATION OF

Zur Theorie des Durchgangs schneller  
Korpuskularstrahlen durch Materie

by

H. Bethe

Annalen der Physik, Series 5, 5: 325-400, 1930.

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THEORY OF THE PASSAGE OF  
FAST CORPUSCULAR RAYS THROUGH MATTER

by

H. Bethe

The inelastic collision of a fast charged particle (electron, proton,  $\alpha$ -particle) with an atom is treated according to Born's theory of wave mechanics. A very simple procedure is given for evaluating the matrix elements involved in the theory (section 3) and the close relationship to the intensity of the Compton effect is determined (section 5). The theory is developed in detail for collisions of hydrogen atoms and, in as far as possible, for complex atoms. The following are computed: the angular distribution of the inelastically (sections 6, 7, and 17) and elastically (section 16) scattered particles, the excitation cross sections for the excitation of the optical (sections 9 and 17) and x-ray (section 15) levels by electron collision, the sum of all inelastic and elastic collisions, and also the number of the primarily (sections 10 and 18) and secondarily (section 19) formed ions, the velocity distribution of the secondary electrons (section 18) and, finally, the braking of the colliding particles by gas atoms (sections 10, 12, and 13). The agreement of this theory with experiment is satisfactory to good. (For more detail see the summary in section 20).

I. GENERAL

1. Introduction

Essentially three types of processes take place during the passage of electrons through matter:

1. Elastic collisions: directional change of the electron without appreciable \*) change of its velocity, no change of the excitation state of the atom. The elastically scattered electrons are capable of interference.

---

\*) Of course, during collision with an atom at rest there is always a small decrease in velocity according to the law of energy momentum.

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2. Inelastic collisions: braking and generally minor changes (cf. section 6) in direction of the electron accompanied by excitation or ionization of the atom that has experienced collision. The inelastically scattered electrons are not capable of interference.

3. Bremsung of the electron with emission of wave radiation (x-ray bremsung spectrum).

There is analogy to all three processes in the interaction of light and matter, namely:

1. coherent scattering capable of interference without change in wavelength,
2. incoherent scattering, generally with an increase in wavelength (Raman or Compton effect),
3. photoeffect, i. e., absorption of wave radiation with acceleration of an electron from an atom.

Here, the analogy between fast electrons and shortwave light is quite close: The number of elastic electron collisions is closely related to the intensity of the coherently scattered x-rays of the same wavelength (cf. ref. [1], section 8 and refs. [2-4]), and the number of inelastic collisions is also closely related to the intensity of the scattering with a change in wavelength (cf. section 5).

$\alpha$ -rays also experience elastic and inelastic collisions in passing through matter, but because of their large mass, bremsung with emission of wave radiations is only of minor importance. Instead, the possibility exists that an electron will be captured from an atom. This "charge exchange" of the  $\alpha$ -particles has been treated satisfactorily by Oppenheimer [5] on the basis of quantum mechanics; in this paper we shall disregard both this charge exchange and the emission of x-ray bremstrahlung and limit ourselves to the theory of elastic and, especially inelastic collisions, deceleration<sup>\*)</sup> of the colliding particle caused by

<sup>\*)</sup> Although we neglect emission of the x-ray bremsung here, we should get nearly the total bremsung, because the energy used in the emission of the x-ray bremsung spectrum is very small (approximately 1/1000 of the kinetic energy of the particles).

these collisions, and excitation and ionization of the atoms by the colliding particle.

Theories are plentiful for this case as well. They are developed either on a purely classical basis, e.g., Bohr [6, 7], or they make some use of quantum-theoretical points of view [8-11]. However, in all these papers \*) rather arbitrary assumptions had to be made about the interaction between the colliding particle and the atom. Therefore it seemed expedient, in view of the numerous experimental works in this field, to develop Born's strictly wave-mechanical collision theory [12] as extensively as possible. This lead to results that differ somewhat \*\*) from those of the classical theory but which are more precise in any event. Further, computation is far simpler than by the classical method in its familiar form: Wave mechanics yields the desired information, i.e., the statistics of the collision process, immediately, without first introducing a collision parameter in addition to the physically significant magnitudes and only then averaging over all the values of this parameter.

The present theory is limited to the case of high velocity of the colliding particle (only in this case does Born's collision theory yield a dependable result, even in the first approximation which was employed here). For, as Distel of this institute will show in his paper (soon to be published), the Born process is a development by descending powers of  $v^2/v_0^2$ , where  $v$  is the velocity of the particle and  $v_0$  the velocity of an electron in a "Bohr orbit" of the atom. The process, therefore, does not converge any better, e.g., for  $\alpha$ -particles with a certain velocity than for electrons with the same velocity. In general, in analogy to optics, one would sooner expect a development according to descending powers of the wave number, or, perhaps even development according to descending powers of the kinetic energy. Thus, we always presuppose  $v \gg v_0$ .

\*) Except for Elsasser, who uses Born's collision theory as do we. However, his computations for the scattering of fast particles have not been carried out explicitly. His derivation may also be simplified essentially.

\*\*) Contrary to Gaunt's opinion (cf. [10]).

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## 2. Notation

We shall use the following notation consistently:

$a$  = radius of the innermost Bohr orbit in the hydrogen atom

$$a = \frac{1}{a}, \quad a_0 = \frac{2\pi}{\hbar} \sqrt{-2mE_0}, \quad a_n = \frac{2\pi}{\hbar} \sqrt{-2\pi E_n},$$

$$a_{0,n} = \sqrt{a_0^2 - a_n^2} \quad [\text{vgl. (12)}], \quad a_{n,l} = \frac{2\pi}{\hbar} \sqrt{-2\pi E_{n,l}}.$$

$E_n$  = energy (eigenvalue) of the  $n^{\text{th}}$  atomic state

$E_0$  = eigenvalue of the ground state

$E_{nl}$  = eigenvalue (negative ionization potential) of the  $(nl)$ -shell

$\epsilon_n$  = matrix element, corresponding to the transition from the ground state to the  $n^{\text{th}}$  excited state; for definition, cf. (11)

$\epsilon_{nl, n'l'}$  = matrix element, corresponding to the transition of an electron from the  $nl$ -shell to the  $n'l'$ -shell

$dE(q)$  = the energy transferred to the atom from the particle during collision with a change in momentum between  $q$  and  $q + dq$ .

$E$  = total energy transferred to the atom per unit time

$f_{m,n}$  = generalized oscillator strength, corresponding to the transition from atomic state  $m$  to state  $n$  (definition (45))

$f_{nl, n'l'}$  = oscillator strength, corresponding to the transition of an electron from the  $nl$ -shell to the  $n'l'$ -shell (definition (61a))

$f_{nl} = \sum_{n'l'} f_{nl, n'l'} =$  sum of the oscillator strengths for all transitions of an electron of the  $nl$ -shell (cf. (62))

$F$  = atomic form factor of the x-ray scattering theory

$d\Phi(q)$  = differential effective cross section = number of collisions with transfer of momentum between  $q$  and  $q + dq$  (section 7)

$\Phi$  = integral effective cross section for all inelastic collisions (section 10)

$\Phi_n$  = integral effective cross section for excitation of the  $n^{\text{th}}$  atomic state (section 3 ff., section 9)

$\Phi_{nl}$  = effective cross section for the transition of an electron  $n'l'$  from the  $nl$ -shell into the  $n'l'$ -shell (cf. section 14)

$\Phi^{nl}$  = effective cross section for all possible excitations of an  $nl$ -electron (cf. section 15)

$\varphi_n$  = generalized transition probability (definition (34))

$\mathbf{g} = \frac{2\pi}{\hbar} \mathbf{M}\mathbf{v}$  = propagation vector of the de Broglie wave of the motion of the particle with respect to the atom before collision

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$\mathbf{R} = \frac{2\pi}{\hbar} M \mathbf{v}'$  = propagation vector after collision

$K = |\mathbf{R}|$ ,  $K' = |\mathbf{R}'|$  = wave numbers of the colliding particle

$k$  = wave number of the secondary electron

$l$  = azimuthal quantum number

$\lambda = \frac{\hbar}{mv} = \frac{2\pi}{K}$  = wavelength of the de Broglie wave of the colliding particle

$m$  = mass of the electron

$M_1$  = mass of the colliding particle

$M_2$  = mass of the atom which has been struck

$M = \frac{M_1 M_2}{M_1 + M_2}$  = effective mass of the colliding particle

$\mathbf{q} = \mathbf{R} - \mathbf{R}' = \frac{2\pi}{\hbar} M (\mathbf{v} - \mathbf{v}')$  = collision vector = (geometric) change of the momentum of the colliding particle in units  $\hbar/2\pi$ ,  $q = |\mathbf{q}|$

$\mathbf{r}$  = position vector of the colliding particle, reckoned from the nucleus of the struck atom

$\mathbf{r}_j$  = position vector of the  $j^{\text{th}}$  electron

$s_0$  = number of the primarily formed ions per centimeter of path

$s$  = number of all ions formed per centimeter of path

$T = \frac{M_1 v^2}{2}$  = kinetic energy of the particle

$T_r = \frac{M}{2} v^2$  = kinetic energy of the motion of the particle relative to the atom

$d\tau_{\mathbf{R}}$  = volume element in the space of the colliding particle

$d\tau_j$  = volume element in the space of the  $j^{\text{th}}$  electron,  $d\tau = \prod_j d\tau_j$

$u$  = time dependent wave function of the total system (atom + colliding particle)

$v$  = velocity of the particle before the collision,  $v = |\mathbf{v}|$

$v'$  = velocity after collision,  $v' = |\mathbf{v}'|$

$ze$  = charge of the colliding particle

$Ze$  = charge of the atomic nucleus

$Z_{nl}$  = number of electrons in the  $nl$ -shell

$\Psi_n$  = eigenfunction of the atom in the  $n^{\text{th}}$  state

$\psi_{nl}$  = eigenfunction of an electron in the  $nl$ -shell ( $n$  = principal quantum number,  $l$  = azimuthal quantum number)

$\psi_k$  = continuous eigenfunction of an electron (wave number  $k$ )

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### 3. General Scattering Formula

Neglecting the interaction between a colliding particle and an atom, the wave function of the system atom + particle is

$$u_0 = \sqrt{\frac{2\pi M}{\hbar K}} e^{i(\vec{K} \cdot \vec{R})} \psi_0(\vec{r}_j) e^{-\frac{2\pi i}{\hbar} W t} \quad (1)$$

$$W' = \frac{\hbar^2}{8\pi^2 M} K'^2 + E_0.$$

Expression (1) is normalized such that one particle passes through the unit surface per unit time. If the "interaction" is "switched on" at time  $t = 0$ , the wave function at time  $t$  can be expanded over the eigenfunctions  $\chi$ , without interaction (method of variation of the constants):

$$u(t) = \sum_{n, \vec{R}'} a_n(\vec{R}', t) \chi_n(\vec{R}; \vec{R}', \vec{r}_j) \quad (2)$$

$$\chi_n(\vec{R}') = \sqrt{\frac{MK'}{2\pi\hbar^2}} e^{i(\vec{R}' \cdot \vec{R})} \psi_n(\vec{r}_j) e^{-\frac{2\pi i}{\hbar} W' t} \quad (3)$$

$$W' = E_n + \frac{\hbar^2}{8\pi^2 M} K'^2.$$

Expression (3) is normalized per energy interval  $dW' = \frac{\hbar^2}{4\pi^2 M} K' dK'$  and per solid angle element  $d\omega'$  (relative to the velocity and direction of the particle after collision). Coefficients  $a_n(\vec{R}')$  in (2) are obtained from the time-dependent Schrödinger equation to a first approximation ( $V$  is the interaction energy):

$$\frac{\hbar}{2\pi i} \cdot \frac{da_n(\vec{R}' t)}{dt} = \int V u_0 \bar{\chi}_n(\vec{R}') d\tau \cdot d\tau_R \cdot$$

$$- \frac{2\pi i}{\hbar} (W - W') \cdot -1 \sqrt{\frac{MK'}{\hbar^2 K}} e^{\frac{2\pi i}{\hbar} (W - W') t} \quad (4)$$

$$\left\{ \begin{aligned} V_{on}(\vec{R}, \vec{R}') &= V_{on}(q) = \int \left( \frac{Z}{|\vec{R}'|} - \sum_{j=1}^Z \frac{1}{|\vec{R} - \vec{r}_j|} \right) \\ &\quad \cdot \psi_0(\vec{r}_j) \bar{\psi}_n(\vec{r}_j) e^{i(\vec{R} - \vec{R}', \vec{R})} d\tau \cdot d\tau_R. \end{aligned} \right. \quad (5)$$

If we proceed to large times  $t$ , the energy theorem

$$W = W' = E_0 + \frac{\hbar^2}{8\pi^2 M} K'^2 = E_n + \frac{\hbar^2}{8\pi^2 M} K'^2 \quad (6)$$

will be satisfied to a significant degree, and by integration of  $|a_n(\vec{R}')|^2$  over a certain energy interval  $\Delta W' \gg \frac{\hbar}{2\pi t}$  and by differentiation of the

integral with respect to time we obtain, in the familiar manner, the transition probability to the  $(n, R')$ -state, i.e., the number of particles that are scattered per unit time in direction  $R'$  and thereby excite the atom to the  $n^{\text{th}}$  quantum state:

$$\begin{aligned} d\Phi_n(q) &= d\omega \frac{d}{dt} \int dW' |a_n(R', t)|^2 \\ &= \frac{4\pi^2}{\hbar} \cdot \frac{M^2 K'}{\hbar^2 K} \cdot 2\pi \sin \vartheta d\vartheta \cdot e^4 z^3 \cdot |V_{n,n}(q)|^2 \\ d\Phi_n(q) &= \frac{1}{2\pi} \alpha^2 \left(\frac{M}{m} z\right)^3 \sin \vartheta d\vartheta |V_{n,n}|^2 \frac{K}{K'} \quad (7) \end{aligned}$$

$d\Phi_n(q)$  has the dimension of a surface (number of collisions per unit time in the flow of a particle through the unit surface per unit time). It means the effective cross section of the atom for scatterings at the angle  $\vartheta$  with simultaneous excitation of the  $n^{\text{th}}$  atomic state, which we shall define as the differential effective cross section.

Usually, the matrix elements  $V_{0n}$  of the interaction energy are now evaluated by integrating first over the coordinates of the atomic electron and only then over those of the colliding particle [13] or else, by expanding  $e^{i(R-R', R)}$  according to spherical functions and then by finishing the integrations over the angular coordinates, and next the radial integrations [11].

The following method is much simpler and also demonstrates directly the relation to x-ray scattering:

First, we integrate over the space of the particle and note that, e.g.,

$$\varphi_q(r_j) = \int \frac{1}{|R - r_j|} e^{i(q \cdot R)} d\tau_R \quad (8)$$

is the potential of a charge distributed with density

$$\rho_q(R) = e^{i(q \cdot R)} \quad (8a)$$

at the point  $r_j$ . However, from

$$d\varphi_q(r) = -4\pi\rho = -4\pi e^{i(q \cdot r)} \quad (8b)$$

(9)

$$\varphi_q(r) = \frac{4\pi}{q^2} e^{i(q \cdot r)}.$$

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follows directly, i. e., the differential effective cross section becomes

(10)

$$d\Phi_n(q) = \frac{8\pi a^3}{q^4} \left( \frac{M}{m} z \right)^2 \frac{K'}{K} |\psi_n(q)|^2 \sin \theta d\theta$$

with

$$\psi_n(q) = \int \left( Z - \sum_j e^{i(q r_j)} \right) \Psi_0 \bar{\Psi}_n(r_j) \prod_j dr_j, \quad (11)$$

where we need only to integrate over coordinates of the atomic electrons.

The step (8) to (9) may seem somewhat bold, since the integral in (8) does not converge. In fact, if we set  $r = R - r_j$  and introduce a system of polar coordinates with the axis  $q$ , we will have

$$\begin{aligned} \varphi_q(r_j) &= e^{i(q r_j)} \int_0^\infty r^2 dr \int_0^\pi 2\pi \sin \theta d\theta \cdot \frac{1}{r} e^{iqr_j \cos \theta} \\ &= \frac{4\pi e^{i(q r_j)}}{q} \int_0^\infty \sin qr_j dr. \end{aligned}$$

However, we can easily obtain convergence in the usual manner by letting the value  $q$  of the collision vector pass through a certain range  $q - \Delta q$  to  $q + \Delta q$  and averaging  $\varphi_q$  over this range, and also by reversing the integrations over  $q$  and  $r$ :

$$\begin{aligned} &\lim_{\Delta q \rightarrow 0} \frac{1}{2\Delta q} \int_{q-\Delta q}^{q+\Delta q} dq' \varphi_{q'}(r_j) \\ &= \lim_{\Delta q \rightarrow 0} \frac{4\pi e^{i(q r_j)}}{2q \Delta q} \int_0^\infty dr \int_{q-\Delta q}^{q+\Delta q} \sin q' r dq' \\ &= \lim_{\Delta q \rightarrow 0} \frac{4\pi e^{i(q r_j)}}{2q \Delta q} \int_0^\infty \frac{dr}{r} (\cos(q - \Delta q)r - \cos(q + \Delta q)r) \\ &= \lim_{\Delta q \rightarrow 0} \frac{4\pi e^{i(q r_j)}}{2q \Delta q} \ln \frac{q + \Delta q}{q - \Delta q} = \frac{4\pi e^{i(q r_j)}}{q^2}. \end{aligned}$$

Thus formula (10) is justified. This will be discussed in section 5.

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#### 4. Energy Relationships

First we must consider the relationships implied by energy theorem (6) among the collision vector  $q$ , the scattering angle  $\vartheta$ , and the excitation energy transferred to the atom:

$$E_n - E_0 = \frac{h^2}{8\pi^2 m} (a_0^{-2} - a_n^{-2}) = \frac{h^2}{8\pi^2 m} a_{0n}^2. \quad (12)$$

The reciprocal lengths  $a_0$ ,  $a_n$ , and  $a_{0n}$  defined by (12), are of the order of magnitude of the reciprocal atomic radius ( $10^8 \text{ cm}^{-1}$ ) for discrete atomic states  $n$ . With excitation to a state  $k$  of the continuous spectrum (ionization),  $-a_n^{-2}$  must be replaced by  $k^2$  (wave number of the secondary electron) and (12a)

$$E_k - E_0 = \frac{h^2}{8\pi^2 m} (a_0^{-2} + k^2). \quad (12a)$$

The energy theorem (6) requires

$$K^2 - K'^2 = \frac{M}{m} a_{0n}^2. \quad (13)$$

By definition

$$q = \vec{R} - \vec{R}' \quad (14)$$

$$q^2 = K^2 + K'^2 - 2KK' \cos \vartheta,$$

i.e.,

$$q^2 = 2K^2 - \frac{M}{m} a_{0n}^2 - 2K \sqrt{K^2 - \frac{M}{m} a_{0n}^2} \cos \vartheta. \quad (14a)$$

For elastic collisions ( $E_n = E_0$ ,  $a_{0n} = 0$ ) this is identical to

$$q = 2K \sin \frac{\vartheta}{2} = \frac{4\pi \sin \frac{\vartheta}{2}}{1} = \frac{4\pi M}{h} v \sin \frac{\vartheta}{2}. \quad (14b)$$

Indeed, this magnitude is known from the theory of x-ray scattering, in which the scattering intensity at the angle  $\vartheta$  is a function of this magnitude.

With constant excitation energy,

$$\sin \vartheta d\vartheta = \frac{q dq}{KK'} . \quad (15)$$

results from (14). It can be seen that when (15) is introduced into (10),

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the wave number  $K'$  of the particle is completely eliminated after the collision:

$$d\Phi_n(q) = \frac{8\pi n^2}{K^2} \left( \frac{M}{m} z \right)^2 \frac{dq}{q^3} |\epsilon_n(q)|^2. \quad (16)$$

Thus, if the differential effective cross section is conceived of as the number of particles whose momentum during collision experiences a change between  $\frac{h}{2\pi}q$  and  $\frac{h}{2\pi}(q + dq)$  rather than the number of particles deflected into a certain solid angle element  $d\Omega \sin\vartheta$ , the effective cross section will be a function of the excitation of the atom produced by the collision only by virtue of the matrix element  $\epsilon_n(q)$ . This considerably facilitates the formation of the total cross section by integration over  $\vartheta$  or  $q$  (sections 7 and 8). In view of this anticipated integration, we now determine the limits of integration:

1. The smallest possible collision vector  $q_{\min}$  (scattering angle  $\vartheta = 0$ ) depends (cf. (14a)) on the excitation energy  $E_n - E_0$ . As long as this excitation energy is of the order of magnitude of the ionization potential, i. e., as long as either a discrete atomic state is excited, or, in the case of ionization, only a small kinetic energy (i. e., of the order of magnitude of the ionization potential) is imparted to the detached secondary electron,  $K \gg a_{0n} \frac{M}{m}$  is surely valid and because  $M \geq m$ ,  $K^2 \gg \frac{M}{m} a_{0n}^2$ . We had to assume (see end of section 1) that the velocity  $v = \frac{hK}{2\pi M}$  of the particle is large versus the velocity of an electron in a Bohr orbit of the atom, which must be defined analogously by the expression  $v_0 = \frac{ha_0}{2\pi m}$ , to permit us to operate solely with the first approximation of the Born procedure. Thus, in (14a) we can expand over

$$\frac{M a_{0n}^2}{m K^2} = \frac{E_n - E_0}{T_r}$$

and get

$$q^2 = \left( 2K^2 - \frac{M}{m} a_{0n}^2 \right) (1 - \cos \vartheta) + \frac{1}{4} \left( \frac{M a_{0n}^2}{m K} \right)^2 \cos^2 \vartheta + \dots \quad (17a)$$

$$q_{\min} = q_{\vartheta=0} = \frac{M a_{0n}^2}{2m K}. \quad (17)$$

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$$\text{Because } K \gg \frac{M}{m} a_{0n},$$

$$q_{\min} \ll a_{0n},$$

holds, and  $q_{\min}$  decreases with the transferred excitation energy and decreases with increasing velocity of the particle (as in ref. [11, p. 537]).

2. For the overwhelming majority of collisions with a small collision vector  $q$ , the above assumption that the energy transfer is approximately equal to the ionization potential and, therefore, is small relative to the kinetic energy of the particle is certainly correct (cf. section 6). The most common inelastic collisions with a large  $q$  (i. e., with a large deflection of the colliding particle), however, are those in which the momentum theorem is almost satisfied for the colliding particle and the secondary electrons. Except for the factor  $h/2\pi$ ,  $q$  is the change of momentum of the colliding particles, thus the momentum of the secondary electron must be almost  $\frac{h}{2\pi} q$  with a wave number  $k \approx q$ . Then, since  $a_0 \ll q$ ,  $a_{0n}$  is also approximately equal to  $q$  and, by substitution in (18a), we obtain

$$\left\{ \begin{aligned} \cos \delta' &= \frac{K^2 + K'^2 - q^2}{2KK'} = \frac{K^2 \left(1 - \frac{m}{M}\right) + K'^2 \left(1 + \frac{m}{M}\right)}{2KK'} \\ &= \frac{2K^2 - q^2 \left(1 + \frac{M}{m}\right)}{2K \sqrt{K^2 - q^2 \frac{M}{m}}} . \end{aligned} \right. \quad (18)$$

for the angle  $\delta'$  between the azimuths of the colliding particle before and after the collision. The same applies to the angle  $\varphi$  between the direction  $q$  of the secondary electron and the original azimuth  $\theta$  of the primary electron according to the cosine law

$$\cos \varphi = \frac{K^2 + q^2 - K'^2}{2Kq} = \frac{q \left(1 + \frac{M}{m}\right)}{2K} . \quad (18a)$$

a) If the colliding particle is an electron, because  $M = m$ , we get

$$q = K \sin \theta = K \cos \varphi, \quad K' = K \cos \theta. \quad (19)$$

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This is the law of classical theory [14] which states that after collision the azimuths of the primary and secondary electrons are perpendicular to each other. The greatest possible scattering angle  $\delta_{\max}$  is  $90^\circ$  and the maximum collision vector  $q_{\max} = K$ .

b) If the colliding particle is a heavy ( $\alpha$  or H) particle,  $M \gg m$ . Then, it follows from (18a) that with a small transfer of momentum the secondary electron leaves the atom perpendicularly to the direction of the  $\alpha$ -particle, while with a larger collision vector  $q$  it receives an increasing momentum component in the primary direction. The greatest possible collision vector results when the electron is ejected along the continuation of the path of the oncoming particle ( $\varphi = 0$ ), in which case

$$q_{\max} = 2K \frac{m}{M+m} \approx 2K \frac{m}{M}, \quad (20)$$

i.e., the secondary electron precedes the  $\alpha$ -particle with the velocity  $\frac{hq}{2\pi m} \approx 2 \times \frac{hK}{2\pi M} = 2v$ . This, of course, is in full agreement with the result of classical theory, which was indeed based on the law of energy momentum. The angle of deflection  $\delta$  of the colliding particle varies only within a very small range: \*) when the transferred momentum

grows from 0 to  $\frac{q_{\max}}{\sqrt{2}}$  (and  $\varphi$  decreases from  $90^\circ$  to  $45^\circ$ ), the scattering angle increases from 0 to  $\delta_{\max} = \arcsin \frac{m}{M}$ , only to decrease again to zero during a further increase of the momentum transfer to  $q_{\max}$ .

The energy loss  $E_n - E_0$  of the colliding particle by excitation or ionization of the atom, discussed so far, refers only to the decrease of the relative velocity of the colliding particle to the atom from  $v$  to  $v'$  ("collision with the electrons of the atom" in classical theory). However, if the atom was initially at rest, this is no longer the case after the collision, and, consequently, the energy decrease of the colliding particle is somewhat greater still in a system at rest: A transfer of kinetic energy from the particle to the atom occurs according to the classical law of energy momentum. The velocity

$$\frac{M_1}{M_1 + M_2} v$$

\*) According to the sine law,  $\sin \delta / \sin \varphi = q/K'$ .

of the center of gravity of atom and colliding particle relative to a system at rest and the [velocity]

$$\frac{M_1}{M_1 + M_2} \mathbf{v}'$$

of the particle relative to the center of gravity, are added vectorially to constitute the particle velocity  $\mathbf{v}''$  after the collision in a system at rest:

$$\begin{aligned} v''^2 &= \frac{1}{(M_1 + M_2)^2} (M_1^2 v^2 + M_2^2 v'^2 + 2M_1 M_2 v v' \cos \theta) \\ &= v^2 - \frac{M_1 M_2}{(M_1 + M_2)^2} (v^2 + v'^2 - 2v v' \cos \theta) \\ &\quad - \frac{M_2}{M_1 + M_2} (v^2 - v'^2). \end{aligned}$$

The total loss of kinetic energy in a system at rest is, therefore,

$$\left\{ \begin{aligned} \frac{M_1}{2} (v^2 - v''^2) &= \frac{M_1}{M_1 + M_2} \cdot \frac{M}{2} \cdot |v - v'|^2 + \frac{M}{2} (v^2 - v'^2) \\ &= \frac{M_1}{M_1 + M_2} \cdot \frac{\hbar^2}{8\pi^2 M} q^2 + \frac{\hbar^2}{8\pi^2 M} (K^2 - K'^2) \\ &= \frac{\hbar^2}{8\pi^2 M_2} q^2 + E_n - E_b. \end{aligned} \right. \quad (21)$$

As we have seen, the second term, the transferred excitation energy is of the order of magnitude of  $\frac{\hbar^2}{2} q^2$  (in the case of large  $q$ ) or  $\frac{\hbar^2}{8\pi^2 m} a_0^2$  (when  $q \ll a_0$ ), i.e., the first term is always smaller than the second by at least the factor  $m/M_2 = \frac{\text{electron mass}}{\text{atomic mass}}$ , just as in classical theory the energy loss due to the scattering on the nucleus is smaller than the loss due to the scattering on the electrons.

### 5. Collisions and X-Ray Scattering

Now we shall discuss the formula (10), or (16), for the differential effective cross section and relate the latter to the intensity of x-ray scattering:

1) For elastic collisions, we get (cf. (11))

$$\epsilon_0(\eta) = Z - \int \sum_i e^{i(\eta \tau)} |\Psi_0|^2 d\tau = Z - F. \quad (22)$$

That is, the following theorem holds with respect to (14b):

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The effective cross section for elastic collisions at a definite deflection angle  $\vartheta$  is

$$d\Phi_0(q) = \frac{2\pi e^4 Z}{16 T_r^4} \frac{(Z - F)^2}{\sin^4 \frac{\vartheta}{2}} \sin \vartheta d\vartheta, \quad (23)$$

where  $Z$  is the atomic number and  $F$  the atomic form factor (dependent on  $q$ ) of the theory of x-ray scattering. The elastic scattering of corpuscular particles differs from that of x-rays by the addition of the "scattering by the nucleus" to the "scattering by the electron cloud of the atom" ( $Z - F$  instead of  $F$ ) and by the characteristic factor

$$\frac{1}{\sin^4 \frac{\vartheta}{2}}$$

of Rutherford's formula.

2) For inelastic collisions, the "scattering by the nucleus"

$$\int Z \Psi_0 \bar{\Psi}_n d\tau$$

vanishes, owing to the orthogonality of the eigenfunctions; we get

$$-e_n = \sum_j \int e^{i(\mathbf{q} \cdot \mathbf{r})} \Psi_0 \bar{\Psi}_n(\mathbf{r}_j) d\tau \quad (24)$$

equal to the matrix element [15 et alibi, 16] critical for the incoherent x-ray scattering (Compton effect).

The differential effective cross section for inelastic collisions, except for the "Rutherford factor"  $1/\sin^4 \frac{\vartheta}{2}$ , is proportional to the intensity of the Compton scattering of x-rays. Here, collisions with identical change of momentum  $\frac{h}{2\pi} q$  (of the particle or the light quantum) must be compared. (In a region of medium angles,  $q$  is proportional to  $\sin \vartheta/2$ . \*)

3) When the angles of deflection are small and the energy transfer to the atom  $E_n - E_0$  is not too large, the collision vector  $q$ , as noted in (17a) and (17), is small compared with the "reciprocal

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<sup>\*)</sup> That is, when (17a) still holds (i.e.,  $q \ll a_0$ ) but the first term of (17) predominates, viz.,  $q \gg q_{\min} \approx a_0^2 / 2K \times M/m$ .

atomic radius." In this case, which includes most collisions, we may expand the exponential functions in (11) or (24)

$$e^{i(qz)} = e^{iz}, = 1 + iq z_i \pm \dots$$

because of the factor  $1/q^4$  in (10) for the differential collision cross section, and break them off after the first term. Then

$$\epsilon_n(q) = iq \int_j x_j \psi_0 \bar{\psi}_n(r_j) d\tau \quad (25)$$

holds, where  $\left\{ \begin{array}{l} d\psi_n(q) = \frac{8\pi a^3}{q^4} \left( \frac{M}{m} z \right)^2 \frac{K'}{K} \sin \theta d\theta \cdot q^2 \cdot |x_{0n}|^2 \\ = \frac{8\pi a^2}{K^2} \cdot \left( \frac{M}{m} z \right)^2 |x_{0n}|^2 \frac{dq}{q}, \\ x_{0n} = \int_j x_j \psi_0 \bar{\psi}_n(r_j) d\tau \end{array} \right. \quad (26)$

is the matrix element of the sum of the electron coordinates (or that of the electric moment of the atom). Thus, for small collision vectors  $q$  (i.e., small changes in momentum of the colliding particle), the collision probability is proportional to the square of the coordinate matrix, i.e., proportional to the optical transition probability for the respective excitation of the atom<sup>\*)</sup> and, because of  $1/q$ , the integral collision cross section also becomes almost proportional to this magnitude (cf. sections 9 and 14).

## II. COLLISION WITH HYDROGEN ATOMS

### 6. Evaluation of the Matrix Elements

In a study of the Compton effect, Wentzel evaluated the matrix elements  $\epsilon_n(q)$  that enter into the differential effective cross section (20) and are defined by (11) for transitions from the ground state of the hydrogen atom to the states of the continuous spectrum in a parabolic coordinate. Here, it must be noted that a continuous group of eigenfunctions  $\psi_{km}$ , belonging to a definite continuous eigenvalue

$$E_k = \frac{\hbar^2}{8\pi^2 m} k^2$$

<sup>\*)</sup>This theorem has already been derived for hydrogen by Elsasser [11, pp. 537, 538], who also presumed it to be universally valid.

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differ in their parabolic quantum numbers  $m$ . Hence, the square of the matrix element (normalized per  $dk$ ) becomes, for the transition from the ground state to the  $E_k$  state (cf. [15, p. 365]),

$$|\epsilon_k(q)|^2 = \int_{-\infty}^{+\infty} dm |\epsilon_{0,k_m}(q)|^2 \quad (27)$$

By elementary evaluation of Wentzel's formula (28), and taking his formulas (27), (25), and (19) into account, we obtain,<sup>\*)</sup>

$$\left\{ \begin{array}{l} |\epsilon_{0,k_m}(q)|^2 = \frac{256 k^2 q^2 m^2 c^{-2} \frac{a}{k} \operatorname{arctg} \frac{2\pi k}{q^2 - k^2 + a^2}}{(q + k)^2 + a^2 [(q - k)^2 + a^2]} \cdot a(m) \\ a(m) = \frac{q^2 + 4k^2 m^2}{(1 + e^{-2\pi(n+m)})(1 + e^{-2\pi(n-m)})}, \quad n = \frac{a}{2k}. \end{array} \right. \quad (28)$$

The integration over  $m$  anticipated in (27)

$$|\epsilon_k(q)|^2 = c(k, q) \int_{-\infty}^{+\infty} a(m) dm \quad (28a)$$

requires evaluation of integrals of the type

$$J_\mu = \int_{-\infty}^{+\infty} \frac{m^\mu dm}{(1 + e^{-2\pi n} \cdot e^{-2\pi m})(1 + e^{-2\pi n} \cdot e^{+2\pi m})} \quad (\mu = 0, 2) \quad (28b)$$

(path of integration is a real axis). This can easily be done with complex terms, in analogy to ref. [15, footnote 2, p. 365]. Thus,

$$\left\{ \begin{array}{l} \int \frac{(m+i)^r dm}{(1 + e^{-2\pi n} \cdot e^{-2\pi(m+i)})(1 + e^{-2\pi n} \cdot e^{+2\pi(m+i)})} \\ \quad - \int \frac{m^r dm}{(1 + e^{-2\pi n} \cdot e^{-2\pi m})(1 + e^{-2\pi n} \cdot e^{+2\pi m})} \\ = \sum_{\mu=0}^{r-1} \binom{r}{\mu} i^{\mu-r} \mu! J_\mu \\ = \oint \frac{m^r dm}{(1 + e^{-2\pi n} \cdot e^{-2\pi m})(1 + e^{-2\pi n} \cdot e^{+2\pi m})} \end{array} \right. \quad (29a)$$

where we have to take the last, closed integral along the real axis from  $+\infty$  to  $-\infty$  and back along the parallel displaced by  $+i$ . Then the two poles

$$m_1 = +n + \frac{i}{2} \text{ with the residue } \frac{-(n + \frac{i}{2})^r}{2\pi(1 - e^{-4\pi n})}$$

$$m_2 = -n + \frac{i}{2} \quad " \quad " \quad " \quad \frac{(-n + \frac{i}{2})^r}{2\pi(1 - e^{-4\pi n})}$$

<sup>\*)</sup> Here  $q$  stands for Wentzel's  $|\Delta k|$ . For hydrogen, the reciprocal radius  $a$  of the innermost Bohr orbit is identical to the  $a_0$  used in section 4 and defined by (12).

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are both circumscribed in the negative direction so that

$$\phi = i \frac{\left(n + \frac{i}{2}\right)^* - \left(-n + \frac{i}{2}\right)^*}{1 - e^{-4\pi n}}. \quad (29b)$$

By using formula (29b) for  $n = 1$  and 3,

$$\begin{cases} J_0 = \frac{2\pi}{1 - e^{-4\pi n}} \\ J_3 = \frac{n}{6} \cdot \frac{-4 + 4n^2}{1 - e^{-4\pi n}} \end{cases} \quad (29c)$$

follows directly from (29a) so that when  $n$  is replaced by its value  $a/2k$ ,

$$|\varepsilon_k(q)|^2 = \frac{2^3 k q^2 a^4 \left(q^2 + \frac{1}{3} (a^2 + k^2)\right)}{[(q + k)^2 + a^2]^2 [(q - k)^2 + a^2]^2} \cdot \frac{e^{-2\frac{\pi}{k} \arctg \frac{3ak}{q^2 - k^2 + a^2}}}{1 - e^{-2\pi \frac{a}{k}}}. \quad (30)^*)$$

For  $q \gg a$ ,  $|\varepsilon_k(q)|^2$  has a sharp maximum at  $k \approx q$  and then passes into the formula derived by Wentzel [15, bottom of p. 365]. For  $q \approx 0$ , (30) becomes  $q^2$  times the usual optical transition probability (square of the element of the coordinate matrix) (cf. section 5, paragraph 3).

$$\begin{cases} \lim_{q \rightarrow 0} |\varepsilon_k(q)|^2 = q^2 |x_{0k}|^2 \\ |x_{0k}|^2 = \frac{2^3}{3} \cdot \frac{a^6 + k^6}{(a^2 + k^2)^2} \cdot \frac{e^{-4\frac{\pi}{k} \arctg \frac{k}{a}}}{1 - e^{-2\pi \frac{a}{k}}} \end{cases} \quad (31)$$

We shall postpone the discussion of (30) and (31) until the end of this section and first evaluate the matrix elements

$$t_n = \int e^{iqz} \psi_0 \bar{\psi}_n d\tau = \frac{3}{\sqrt{2}} \int e^{iqz - ar} \bar{\psi}_n(\xi + \eta) d\xi d\eta \quad (32)$$

for discrete transitions, also in parabolic coordinates

$$x = \frac{1}{2}(\xi - \eta), \quad y = \sqrt{\xi\eta} \cos \varphi, \quad z = \sqrt{\xi\eta} \sin \varphi, \quad r = \frac{1}{2}(\xi + \eta),$$

Here we need consider only eigenfunctions  $\psi_n$  that are independent of  $\varphi$ . These are as follows (cf., e.g., [17, p. 181 ff.]):

$$\psi_n = \frac{1}{\sqrt{2n \cdot n_1! n_2!}} \left(\frac{a}{n}\right)^{\frac{3}{2}} e^{-\frac{a}{2n}(z + \eta)} L_{n_1}\left(\frac{\xi\eta}{n}\right) L_{n_2}\left(\frac{\eta\eta}{n}\right) \quad (32a)$$

$n_1$  and  $n_2$  are the parabolic quantum numbers,  $n = n_1 + n_2 + 1$ . The equation

\*) Read tg as tangent.

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$$\epsilon_{n_1, n_2}(q) = \frac{1}{2^n n! n_1! n_2!} \int e^{-\frac{q^2}{2}} \left(1 + \frac{1}{n} - \frac{i\eta}{a}\right) - \frac{a\eta}{2} \left(1 + \frac{1}{n} + \frac{i\eta}{a}\right) \\ \cdot L_{n_1} \left(\frac{a\eta}{n}\right) L_{n_2} \left(\frac{a\eta}{n}\right) \cdot \alpha(\xi + \eta) \alpha d\xi \alpha d\eta$$

may then be used, for example, by employing the generating function of the Laguerre polynomials: with  $\rho = \frac{a}{n}\xi$  or  $\frac{a}{n}\eta$ ,  $p = n_1$  or  $n_2$ ,  $\beta = 0$  or 1, we have

$$\begin{cases} \sum_p \int \frac{L_p(\rho)}{p!} t^p e^{-\frac{c}{2}(n+1-i\frac{qn}{a})} \rho^p d\rho \\ = \frac{1}{1-t} \int e^{-t\left(\frac{1}{1-t} + \frac{1}{2}(1+n-i\frac{qn}{a})\right)} \rho^p d\rho \\ = (1-t)^{\beta} \beta! 2^{\beta+1} \left[n+1-i\frac{qn}{a} - t(n-1-i\frac{qn}{a})\right]^{-(\beta+1)} \end{cases} \quad (32b)$$

By finding the coefficient  $t^P$  with respect to  $t$  in the expansion of the right side of (32b), we obtain, after short computation,

$$\begin{cases} \epsilon_{n_1, n_2} = \frac{1}{4} n \cdot \frac{\left(n-1-i\frac{qn}{a}\right)^{n_1} \left(n-1+i\frac{qn}{a}\right)^{n_2}}{\left(n+1-i\frac{qn}{a}\right)^{n_1} \left(n+1+i\frac{qn}{a}\right)^{n_2}} \\ \cdot \left( \frac{n_1+1}{n+1-i\frac{qn}{a}} - \frac{n_1}{n-1-i\frac{qn}{a}} + \frac{n_2+1}{n+1+i\frac{qn}{a}} \right. \\ \left. - \frac{n_2}{n-1+i\frac{qn}{a}} \right), \end{cases} \quad (32c)$$

which appears to be very similar to Wentzel's corresponding formula (28) for the transitions to the continuous spectrum, if we also carry out the differentiation with respect to  $a$ . By elementary transformation we obtain

$$\begin{cases} |\epsilon_{n_1, n_2}(q)|^2 = \left(\frac{q}{a}\right)^2 \cdot 2^{\beta} n^{\beta} \cdot \frac{\left[(n-1)^2 + \left(\frac{qn}{a}\right)^2\right]^{n-3}}{\left[(n+1)^2 + \left(\frac{qn}{a}\right)^2\right]^{n+3}} \\ \cdot \left[(n_1 - n_2)^2 + \left(\frac{qn}{a}\right)^2\right]. \end{cases} \quad (32d)$$

Finally, summation over all values possible at the given  $n$ :  $n_1 - n_2 = -n+1, -n+3, \dots, n=3, n-1$ , yields

$$\begin{cases} |\epsilon_n(q)|^2 = \sum_{n_1 + n_2 = n-1} |\epsilon_{n_1, n_2}(q)|^2 = \left(\frac{q}{a}\right)^2 \cdot 2^{\beta} \cdot n^{\beta} \left[ \frac{1}{3} (n^2 - 1) \right. \\ \left. + \left(\frac{qn}{a}\right)^2 \right] \frac{\left[(n-1)^2 + \left(\frac{qn}{a}\right)^2\right]^{n-3}}{\left[(n+1)^2 + \left(\frac{qn}{a}\right)^2\right]^{n+3}} \end{cases} \quad (33)$$

In order to discuss the dependence of the matrix elements  $\epsilon_n(q)$  or the differential effective cross section  $d\Phi_n(q)$  on the collision vector  $q$ , we shall consider the dimensionless magnitude

$$\varphi_n(q) = \frac{a^2}{q^2} |\epsilon_n(q)|^2 \quad (34)$$

and designate it as generalized transition probability; for  $q = 0$ ,  $\varphi_n(q)$  coincides (except for the factor  $a^2$ , introduced to obtain dimensionlessness) with what is usually called the square of the matrix element of the coordinate, since

$$\varphi_n(0) = \frac{2^{\frac{1}{2}} n^2 (n-1)^{3n-6}}{3(n+1)^{2n+5}} \quad (34a)$$

is essentially the familiar intensity formula for the Lyman series. The differential effective cross section is related to the generalized transition probability (cf. (16), (34)) by

$$d\Phi_n(q) = \frac{8\pi}{K^2} \left(\frac{M}{m}\right)^2 \frac{d\eta}{q} \varphi_n(q) \quad (34b)$$

Most of the collisions (55%) at smallest angles ( $q = 0$ ) are those in which the two-quantum level is excited, 17% of all collisions lead to the excitation of higher discrete levels, 28% to ionization. Of the latter, only 4% impart a kinetic energy greater than the simple ionization potential to the secondary electron.

If we proceed to the finite changes of momentum  $q$  of the colliding particle, where  $q$  should still be much smaller than  $a$ , the largest transition probability  $\varphi_2$  decreases somewhat, the transitions to the discrete states with  $n \geq 4$  increase very slightly, ionization increases somewhat more, as may easily be found by logarithmic differentiation of (30) or (33) with respect to  $q$ . If  $q$  acquires the order of magnitude of the reciprocal hydrogen radius  $a$ , all discrete excitation probabilities  $\varphi_n$  decrease greatly, but probabilities of transition  $\varphi_k$  into the continuous spectrum, especially the transfer of greater kinetic energy to the secondary electron, increase. Here, as will be demonstrated in the next section, the sum of all (discrete and continuous) transition probabilities decreases continuously with increasing  $q$ .

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At  $q = 2a$  the discrete transitions comprise only 2% of all transitions; with even greater momentum transfer, excitation of the discrete spectrum is practically precluded. Then, according to (30), the transitions with  $q \approx k$  are by far the most probable, i.e., those transitions for which the secondary electron receives the momentum transferred by the colliding particle (cf. the analogy in the Compton effect [15] et alibi; cf. also section 4 of this paper). The transition matrix is then

$$|\epsilon_k(q)|^2 = \frac{8}{3\pi} \frac{a^4}{[a^2 + (q - k)^2]^3} \quad (34c)$$

as in Wentzel's formula, and decreases essentially with the sixth power of the difference between the momentum of the secondary electron and the change in momentum of the primary electron.

The following table gives the transition probabilities  $\varphi_n(q)$  for some values of  $q$  for the first four discrete transitions and for four selected continuous transitions. The latter are normalized per energy interval; therefore,

$$\frac{\eta_k(q) dk}{k dk} = \frac{\eta_k}{k} = \frac{a^4}{q^4} \frac{|\epsilon_k(q)|^2}{k}.$$

Besides, the sum of all transition probabilities

$$\left\{ \begin{aligned} \varphi(q) &= \sum_n \varphi_n(q) + \int dk \eta_k(q) = \frac{a^4}{q^4} \left( \sum_n |\epsilon_n(q)|^2 \right. \\ &\quad \left. + \int dk |\epsilon_k(q)|^2 \right) \end{aligned} \right. \quad (35)$$

is given, and also the percentage of the discrete transitions in this total probability.

Table I  
Generalized transition probabilities  $\varphi_n$   
from the ground state of hydrogen

	$\frac{q^4}{a^4} = 0$	$\frac{1}{4}$	$\frac{1}{2}$	1	2	4
$n = -2$	0,555	0,328	0,202	0,058	0,0230	0,0034
3	,080	,075	,054	,0267	,0073	,0011
4	,031	,0285	,0218	,0113	,0033	,0005
5	,0145	,0136	,0103	,0058	,0017	,00025
$k = 0$	1,563	1,588	1,300	0,720	0,216	0,032
$\frac{1}{4}$	0,688	0,625	0,914	0,677	,245	,034
1	,116	,193	,276	,374	,278	,039
2	,0017	,0024	,0034	,0062	,0183	,064
$\varphi$	1,000	0,802	0,751	0,500	0,401	0,234

Table 1 (cont.)

Component of the discrete transitions in the total transition probability  $\varphi_n(q)$  in percent

$n =$	2	55,5	38,1	26,0	15,0	5,7	1,45
	3	5,0	8,7	7,2	4,5	1,8	0,47
	4	3,1	3,3	2,9	1,9	0,82	0,20
	5	1,15	1,58	1,45	0,98	0,42	0,11

### 7. Collisions at a Definite Angle

The formula

$$d\Phi_n(q) = \frac{8\pi a^3}{K^2} \left(\frac{M}{m}\right)^2 \frac{dq}{q^2} |\epsilon_n(q)|^2 \quad (16)$$

gives the number of the collisions with a transfer of momentum between  $q$  and  $q + dq$  that lead to the excitation of the  $n$ -quantum state of the atom. The total number of all inelastic collisions with a transfer of momentum between  $q$  and  $q + dq$  may be obtained easily by application of the completeness relation for the eigenfunctions of the hydrogen atom, since

$$\begin{aligned} \epsilon(q) &= \sum_{n=2}^{\infty} |\epsilon_n(q)|^2 + \int dk |\epsilon_k(q)|^2 \\ &= \sum_{n=2}^{\infty} \left| \int e^{iqz} \psi_0 \bar{\psi}_n d\tau \right|^2 + \int dk \left| \int e^{iqz} \psi_0 \bar{\psi}_k d\tau \right|^2 \\ \epsilon(q) &= 1 - F^2, \end{aligned} \quad (36)$$

where \*)

$$F = \int \psi_0^2 e^{iqz} d\tau = \frac{1}{\left(1 + \frac{q^2}{4a^2}\right)^{\frac{1}{2}}} \quad (37)$$

is the atomic form factor for a hydrogen atom in the ground state.

(For the total (generalized) transition probability defined in (35) we

get

$$\begin{cases} \varphi(q) = \frac{a^3}{4} \epsilon(q) = \frac{a^3}{q^2} \left(1 - \frac{1}{\left(1 + \frac{q^2}{4a^2}\right)^2}\right) \\ = \frac{1 + \frac{3}{2} \cdot \frac{q^2}{4a^2} + \left(\frac{q^2}{4a^2}\right)^2 + \frac{1}{4} \left(\frac{q^2}{4a^2}\right)^3}{\left(1 + \frac{q^2}{4a^2}\right)^4} \end{cases} \quad (38)$$

\*) Formula (37), which may be obtained easily, is derived in ref. [1, section 11] together with the atomic form factors of the excited states of the hydrogen atom.

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and by a limiting process (cf. (26), (34))

$$\begin{cases} \varphi(0) = \sum_k \varphi_k(0) + \int dk \varphi_k(0) \\ = a^2 \left( \sum_k |x_{0k}|^2 + \int dk |x_{0k}|^2 \right) = a^2 \int x^2 \psi_0^2 d\tau = 1. \end{cases} \quad (38a)$$

Of course, this last relation may also be derived directly (ref. [1, section 10]). Hence, the effective cross section for all inelastic collisions with a transfer of momentum between  $q$  and  $q + dq$  is

$$d\Phi(q) = \frac{8\pi a^2}{K^2} \left( \frac{M}{m} z \right)^2 \frac{dq}{q^3} (1 - F^2(q)). \quad (39)$$

Correspondingly, the effective cross section for elastic collisions with the same transfer of momentum is, according to (16) and (22),

$$d\Phi_0(q) = \frac{8\pi a^2}{K^2} \left( \frac{M}{m} z \right)^2 \frac{dq}{q^3} (1 - F(q))^2. \quad (40)$$

Of course, formula (39) will not be valid unless the transitions to all quantum states of the discrete and continuous spectrum, or at least all transitions with appreciable transition probability, are actually possible energetically at the given value of  $q$ ; otherwise, the completeness relation must not be used. Therefore, (cf. (17)),

$$q > q_{\min}(k) = \frac{M}{2mK} (a^2 + k^2)$$

must hold for all states  $k$  with appreciable transition probability  $\varphi_k(0)$ , let us say, for all  $k \leq 2a$ , i.e.,

$$q > \frac{5M a^2}{2mK}.$$

Hence, for comparatively fast particles, (39) is valid even for collisions in which  $q$  is much smaller than  $a$ .

1. In the case of scattering at a small angle ( $q \ll a$ ),  $K'$  is almost equal to  $K$  and

$$1 - F = \frac{q^2}{2a^2}, \quad (37a)$$

$$1 - F^2 = \frac{q^2}{a^2}, \quad (37b)$$

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i. e., the effective cross section for inelastic collisions becomes (in view of (15))

$$\left\{ \begin{array}{l} d\Phi(q) = \frac{8\pi}{K^2} \left(\frac{M}{m} z\right)^2 \frac{d\eta}{q} \\ = 8\pi \left(\frac{M}{m} z\right)^2 \frac{\sin \vartheta d\vartheta}{q^3} \approx \frac{8\pi}{K^2} \left(\frac{M}{m} z\right)^2 \frac{d\vartheta}{\sin \vartheta}, \end{array} \right. \quad (39a)$$

and for elastic collisions

$$d\Phi_0(q) = \frac{2\pi}{K^2 a^2} \left(\frac{M}{m} z\right)^2 q dq = 2\pi a^2 \left(\frac{M}{m} z\right)^2 \sin \vartheta d\vartheta. \quad (40a)$$

That is, while the differential effective cross section for elastic collisions approaches a constant boundary value independent of  $\vartheta$  and  $K$ , which is of the same order of magnitude as the gas kinetic cross section, for inelastic collisions the effective cross section increases proportionally to  $1/q^2$  per solid angle element  $\sin \vartheta d\vartheta$  with decreasing scattering angle  $\vartheta$ . Only at very small scattering angles is a boundary value

$$\left\{ \begin{array}{l} \lim_{q \rightarrow 0} d\Phi(q) = 8\pi \left(\frac{M}{m} z\right)^2 \sin \vartheta d\vartheta \cdot \frac{1}{q_{\min}^2}, \\ \approx 8\pi a^2 \left(\frac{M}{m} z\right)^2 \sin \vartheta d\vartheta \left(\frac{m K}{M a}\right)^2 \end{array} \right. \quad (41)$$

reached, which in the ratio  $(\frac{mK}{Ma})^2 = \frac{v^2}{v_0^2}$  is greater than the elastic effective cross section. \*)

2. With scattering at large angles ("single scattering"),  $q \gg a$  and  $F$  is nearly zero (cf. (37)), i. e., the contribution of Schrödinger's density distribution of the atomic electron to the elastic scattering is almost completely canceled by the interference of the contributions of the individual volume elements. Then we get

$$d\Phi_0(q) = d\Phi(q) = \frac{8\pi a^2}{K^2} \left(\frac{M}{m} z\right)^2 \frac{dq}{q^3}. \quad (42)$$

\*) Our formulas (39) ff. are no longer valid for  $\vartheta = 0$ , since at  $\vartheta = 0$   $q$  depends on the excitation energy. However, the first relation (41) is exact when we define

$$\frac{1}{q_{\min}^2} = \sum_n \frac{\varphi_n(0)}{q_{\min}^2(n)} + \int dk \frac{\varphi_k(0)}{q_{\min}^2(k)}$$

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When the transferred momentum is large, elastic and inelastic collisions with identical transfer of momentum occur with the same frequency.

From the standpoint of physics, the number of inelastic collisions with constant transfer of momentum between  $q$  and  $q + dq$  is less interesting than the number of scatterings in a definite angular region from  $\vartheta$  to  $\vartheta + d\vartheta$ . At large scattering angles, for inelastic collisions (cf. section 4)

$$\cos \vartheta = \frac{2 K^2 - q^2 \left(1 + \frac{M}{m}\right)}{2 K \sqrt{K^2 - q^2 \frac{M}{m}}}, \quad (18)$$

is valid for colliding particles of any effective mass  $M$ , or

$$q = K \sin \vartheta, \quad (19)$$

for colliding electrons. For the latter we obtain, from (39) with respect to  $M = m$ ,  $z = 1$  (or directly from (10)),

$$d \Phi(\vartheta) = \frac{8 \pi \alpha^2}{K^4} [1 - F^2(K \sin \vartheta)] \frac{\cos \vartheta d \vartheta}{\sin^3 \vartheta}. \quad (39b)$$

as the effective cross section for inelastic scatterings at angle  $\vartheta$ , while the effective cross section for elastic scatterings is, according to (40) and (14b)

$$\begin{cases} d \Phi_0(\vartheta) = \frac{8 \pi \alpha^2}{K^4} \left[1 - F\left(2 K \sin \frac{\vartheta}{2}\right)\right]^2 \frac{\sin \vartheta d \vartheta}{16 \sin^4 \vartheta/2} \\ = \frac{8 \pi \alpha^2}{K^4} \left[1 - F\left(2 K \sin \frac{\vartheta}{2}\right)\right]^2 \frac{\sin \vartheta d \vartheta}{4(1 - \cos \vartheta)} \end{cases} \quad (40b)$$

For sufficiently large scattering angles, for which  $F \approx 0$ , (40b) becomes the Rutherford formula, and the ratio of inelastic to elastic collisions is

$$\frac{d \Phi(\vartheta)}{d \Phi_0(\vartheta)} = \frac{4 \cos \vartheta (1 - \cos \vartheta)^2}{\sin^4 \vartheta} = \frac{4 \cos \vartheta}{(1 + \cos \vartheta)^2}. \quad (42a)$$

\*)

Elsasser thought that the inelastic scattering (in contrast to the elastic scattering) might disappear at large angles; probably he did not give adequate consideration to transitions into the continuous spectrum.

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$$\text{For } \vartheta = 0^\circ \quad 45^\circ \quad 60^\circ \quad 75^\circ \quad 80^\circ \quad 85^\circ \quad 90^\circ \text{ and more}$$

$$\frac{d\Phi(\vartheta)}{d\Phi_0(\vartheta)} = 1 \quad 0.97 \quad 0.89 \quad 0.65 \quad 0.50 \quad 0.30 \quad 0$$

i.e., the number of elastic and inelastic electron collisions is practically equal at the same scattering angle up to an angle of approximately  $60^\circ$ ; above  $90^\circ$ , there are only elastic collisions (nuclear scattering), because of the approximate validity of the classical law of energy momentum; there are no inelastic ones (collisions with the atomic electrons).

However, in the case of a collision of a heavy particle ( $\alpha$ -particle), only a very small angular region can be involved in inelastic scattering (section 4). Therefore, single scattering (scattering at large angles) is always nuclear scattering (elastic scattering) in this case.\*)

#### 8. Generalized f-Sum Rule

For our subsequent computation of the deceleration of a colliding particle, i.e., the energy per centimeter of path transferred during passage through a gas, let us find not only the number of collisions with a transfer of momentum between  $q$  and  $q + dq$  (cf. section 7), but also the total energy transferred by such collisions to the hydrogen atom through such collisions:

$$dE(q) = \sum_n (E_n - E_0) d\Phi_n(q). \quad (43)$$

Here, the evaluation based on the completeness relation for the eigenfunctions leads to a formula even simpler than that for the number of collisions. For the general case, \*\*) we immediately compute

\*). However, this is due to the approximate validity of the classical law of momentum for colliding particle and secondary electron in theoretical collisions with large transfer of momentum and is, therefore, not a quantum-theoretical phenomenon.

\*\*). Evidently (according to (16)), the equation

$$dE(q) = \frac{8\pi Rh}{K^2} \left( \frac{M}{m} z \right)^2 \frac{dq}{q} f_0(q) \quad (43a)$$

is determined by evaluating (44) in the special case  $m = 0$ . (The sum over  $n$  should also include the continuous spectrum.)

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$$\left\{ \begin{array}{l} f_m(q) = \sum_n f_{mn}(q) = \sum_n \frac{E_n - E_m}{R\hbar} \varphi_{mn}(q) \\ = \frac{a^2}{q^2 R \hbar} \sum_n (E_n - E_m) |\psi_n(q)|^2. \end{array} \right. \quad (44)$$

Since the  $\varphi_{mn}(q)$ 's are generalized transition probabilities, the expression

$$f_{mn}(q) = \frac{E_n - E_m}{R\hbar} \varphi_{mn}(q) = \frac{1}{R} v_{mn} \varphi_{mn}(q) \quad (45)$$

can be defined as the generalized oscillator strength for the transition  $mn$ . For  $q = 0$ , this definition agrees with the definition common in dispersion theory:

$$f_{mn}(0) = \frac{v_{mn} \varphi_{mn}(0)}{R} = \frac{a^2}{R} v_{mn} |x_{mn}|^2 = \frac{8\pi^2 m}{\hbar} v_{mn} |x_{mn}|^2. \quad (45a)$$

In order to evaluate (44), we proceed as when setting up the usual f-sum rule, from the Schrödinger equations

$$\begin{aligned} \Delta \psi_m + \frac{8\pi^2 m}{\hbar^2} (E_m - V) \psi_m &= 0 \\ \Delta \psi_n + \frac{8\pi^2 m}{\hbar^2} (E_n - V) \psi_n &= 0 \end{aligned}$$

with an arbitrary potential  $V$  and only presuppose that  $E_m$  is a discrete eigenvalue, so that from now on we can neglect all surface integrals. Then

$$\left\{ \begin{array}{l} (E_n - E_m) \int \psi_m \bar{\psi}_n e^{iqx} d\tau \\ = \frac{\hbar^2}{8\pi^2 m} \int (\bar{\psi}_n \Delta \psi_m - \psi_m \Delta \bar{\psi}_n) e^{iqx} d\tau \\ = - \frac{\hbar^2}{8\pi^2 m} i q \int \left( \bar{\psi}_n \frac{\partial \psi_m}{\partial x} - \psi_m \frac{\partial \bar{\psi}_n}{\partial x} \right) e^{iqx} d\tau \\ = R\hbar a^2 \left( -2iq \int \frac{\partial \psi_m}{\partial x} \bar{\psi}_n e^{iqx} d\tau \right. \\ \left. + q^2 \int \psi_m \bar{\psi}_n e^{iqx} d\tau \right). \end{array} \right. \quad (45b)$$

$$\begin{aligned} f_m(q) &= \sum_n f_{mn}(q) = \frac{a^2}{q^2 R \hbar} \sum_n (E_n - E_m) \left| \int e^{iqx} \psi_m \bar{\psi}_n d\tau \right|^2 \\ &= \frac{1}{q^2} \sum_n \left( -2iq \int \frac{\partial \psi_m}{\partial x} \bar{\psi}_n e^{iqx} d\tau \right. \\ &\quad \left. + q^2 \int \psi_m \bar{\psi}_n e^{iqx} d\tau \right) \cdot \int e^{-iqx} \bar{\psi}_n \psi_m d\tau \\ &= -2 \frac{i}{q} \cdot \int \frac{\partial \psi_m}{\partial x} \bar{\psi}_n d\tau + \int |\psi_m|^2 d\tau. \\ f_m(q) &= \sum_n f_{mn}(q) = 1. \end{aligned} \quad (46)$$

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The sum of the generalized oscillator strengths  $f_{mn}(q)$  for all transitions from one level of a hydrogen atom is equal to 1, as is the sum of the oscillator strengths  $f_{mn}(0)$ , defined in the usual manner.

Therefore, (43) becomes

$$dE(q) = \frac{8\pi Rh}{K^2} \left(\frac{M}{m} z\right)^2 \frac{dq}{q} = \frac{4\pi e^4 z^2}{m v^2} \frac{dq}{q}. \quad (47)$$

which is the energy transferred by a stream of one particle per unit time and surface per unit time to a hydrogen atom as a result of those collisions in which the momentum of the particle changes by an amount between  $\frac{h}{2\pi}q$  and  $\frac{h}{2\pi}(q + dq)$ . It has the dimension energy times surface.

On the average, during every collision with a change in momentum of the colliding particle between  $q$  and  $q + dq$ , the energy

$$\frac{dE(q)}{d\Phi(q)} = \frac{q^4 R h a^4}{1 - F^2(q)} \quad (48)$$

is transferred, i.e., with large deflections ( $F \approx 0$ )

$$\frac{dE(q)}{d\Phi(q)} = \frac{q^4}{a^2} R h = \frac{h^2}{8\pi^2 m} q^2. \quad (48a)$$

This result is self-evident, since we know that in nearly all cases when  $q$  is large the secondary electron receives the momentum  $\frac{h}{2\pi}q$ , i.e., the energy  $\frac{h^2}{8\pi^2 m} q^2$ . In the case of small deflections we get, according to (37b), simply

$$\frac{dE(q)}{d\Phi(q)} = Rh, \quad (48b)$$

i.e., on the average the simple ionization potential is transferred.

#### 9. Excitation of Certain Energy Levels

We integrate the differential effective cross section over  $\delta$  (or over  $q$ ) and thus obtain the total effective cross section for the excitation of a definite level  $n$ , i.e., the excitation functions for excitation by collision of fast electrons

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$$\Phi_n = \int_{q_{\min}}^{q_{\max}} d\Phi_n(q) = \frac{2^{16} \pi}{3 K^2} \left(\frac{M}{m} z\right)^2 n^7 \cdot A \quad (49)$$

$$A = \int_{q_{\min}}^{q_{\max}} [n^2 - 1 + 3x] \frac{[(n-1)^2 + x]^{n-3}}{[(n+1)^2 + x]^{n+3}} \frac{dx}{x} \quad (49a)$$

by using (33) and (16);  $x = \left(\frac{q n}{a}\right)^2$ . Equation (49a) can be stated in an elementary manner:

$$\begin{aligned} A &= \int [n^2 - 1 + 3x] \sum_{k=0}^{n-3} \binom{n-3}{k} \frac{(-4n)^k}{[(n+1)^2 + x]^{k+1}} \frac{dx}{x} \\ &= \int \frac{dx}{x} [n^2 - 1] c_0' - (n^2 - 1) \sum_{r=0}^{n-2} \frac{c_r' dx}{[(n+1)^2 + x]^{r+1}} \\ &\quad + 3 \sum_{r=3}^{n-2} \binom{n-3}{r-5} (-4n)^{r-5} \frac{dx}{[(n+1)^2 + x]^{r+1}}, \\ c_r' &= \sum_{k=r-5}^{n-3} \binom{n-3}{k} \frac{(-4n)^k}{(n+1)^2 (k+6-r)} \\ &= \frac{(n-1)^2 (n-3)}{(n+1)^2 (n+3-r)} \left[ 1 - \left(\frac{n+1}{n-1}\right)^2 n^{-6} \sum_{k=0}^{r-6} \binom{n-3}{k} \left(\frac{-4n}{(n+1)^2}\right)^k \right]. \end{aligned} \quad (49b)$$

$$\left\{ \begin{array}{l} A = \frac{(n-1)^2 n^{-5}}{(n+1)^2 (n+3)} \left[ \ln x - \ln [(n+1)^2 + x] \right. \\ \quad \left. + \sum_{r=1}^{n-2} \frac{c_{nr}}{r \left(1 + \frac{x}{(n+1)^2}\right)^r} \right]_{q_{\min}}^{q_{\max}}, \end{array} \right. \quad (50a)$$

$$\left\{ \begin{array}{l} c_{nr} = 1 - \left(\frac{n+1}{n-1}\right)^2 n^{-6} \left[ \sum_{k=0}^{r-6} \binom{n-3}{k} \left(\frac{-4n}{(n+1)^2}\right)^k \right. \\ \quad \left. + 3 \binom{n-3}{r-5} \left(\frac{-4n}{(n+1)^2}\right)^{r-5} \frac{n+1}{n-1} \right]. \end{array} \right.$$

Finally, the excitation probability becomes (cf. (34a))

$$\left\{ \begin{array}{l} \Phi_n = \frac{2^{16} \pi}{K^2} \left(\frac{M}{m} z\right)^2 \alpha^2 |x_{0n}|^2 \left[ F_n \left(1 + \left(\frac{n}{n+1} \frac{q_{\max}}{n}\right)^2\right) \right. \\ \quad \left. - F_n \left(1 + \left(\frac{n}{n+1} \frac{q_{\min}}{n}\right)^2\right) \right], \end{array} \right. \quad (50)$$

where

$$F_n(y) = \ln \frac{y-1}{y} + \sum_{r=1}^{n-2} \frac{c_{nr}}{r y^r}. \quad (50b)$$

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In particular:

$$\left\{ \begin{array}{l} F_2(y) = \ln \frac{y-1}{y} + \frac{1}{y} + \frac{1}{2y^2} + \frac{1}{3y^3} + \frac{1}{4y^4}, \\ F_3(y) = F_2(y) - \frac{1}{y^2}, \\ F_4(y) = F_2(y) - \frac{116}{45y^3} + \frac{32}{27y^4}, \\ F_5(y) = F_2(y) - \frac{697}{160y^5} + \frac{85}{24y^6} - \frac{25}{32y^7}. \end{array} \right. \quad (50c)$$

Formulas (50c) completely agree in construction with the formulas given by Elsasser [11, p. 532] for the excitation cross sections of the first transitions. In that respect Elsasser's formulas are somewhat more complete than ours, since he computes the transitions according to partial levels with different azimuthal quantum numbers  $\ell$  separately, while we obtain only the total excitation probability of the levels of the hydrogen atom defined by the principal quantum number  $n$ , because we used parabolic instead of polar coordinates. On the other hand, we have gained so much in simplicity that we can derive the general formula for the effective cross section (50, 50a, 50b) and can easily write the explicit representation of the excitation functions even for higher series terms. \*)

Thus far in this section we have performed Born's approximation without omissions. Now we shall concentrate again on fast particles, introduce for  $q_{\min}$  the value from (17) ( $a_{0n}^2 = a^2(1 - 1/n^2)$  for hydrogen), set  $q_{\max} \approx 2K$  and disregard all powers of  $\frac{aM}{Km} = \frac{v}{v_0}$  beginning with the fourth. We get

$$\Phi_n = \frac{4\pi a^4}{K^2} \left(\frac{M}{m} z\right)^2 |x_{0n}|^2 \ln a_n \left(\frac{2Km}{aM}\right)^2 \quad (51)$$

$$\ln a_n = 2 \ln \frac{n}{n-1} - \sum_{r=1}^{n+3} \frac{c_{nr}}{z}, \quad (51a)$$

$$\Phi_n = \frac{8\pi R \hbar z^4}{m v^2} |x_{0n}|^2 \ln \frac{2a_n m v^2}{R \hbar} \quad (51b)$$

\*) Our formula for  $\Phi_2$  obviously coincides with Elsasser's sum  $\Phi(2,0) + (2,1)$ ; however, the formula for  $\Phi_3$  does not agree with Elsasser's  $\Phi(3,0) + \Phi(3,1) + \Phi(3,2)$ . (Our  $y$  is Elsasser's  $x$ , our  $q_{\max}/a$  his  $S_1$ , and our  $q_{\min}/a$  his  $S_0$ . In his formula for  $F$ , the sign should be reversed.) Since Elsasser's derivation is much more complicated than ours, we are inclined to suspect an error in his formulas.

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$|x_{0n}|^2$  is the square of the coordinate matrix (cf. table 1). For the  $a_n$ 's we get numerically

$$\begin{array}{ccccc} n = & 2 & 3 & 4 & 5 \\ \ln a_n = & -0,697 & -0,272 & -0,115 & -0,042 \\ a_n = & 0,408 & 0,762 & 0,891 & 0,959 \end{array}$$

It now seems that  $\lim_{n \rightarrow \infty} a_n = 1$ .

The excitation cross section is nearly proportional to the optical transition probability and inversely proportional to the square of the velocity of the particle; in addition, there appears - as in Bohr's deceleration theory - a logarithmic term whose argument is proportional to  $v^2$  and in addition is weakly dependent on the level  $n$  which is to be excited. This latter dependence somewhat decreases the excitation cross section for the strongest transitions (small  $n$ 's), although the lower integration limit  $q_{\min}$  in (49a) is lower for these transitions than for those to higher levels.

#### 10. Total Number of Collisions and Deceleration

We now compute the total of all inelastic collisions in general:

$$\Phi = \sum_n \int_{q_{\min}}^{q_{\max}} d\Phi_n(q). \quad (52)$$

We divide the integration into two partial integrations from  $q_{\min}$  to  $q_0$  and from  $q_0$  to  $q_{\max}$ . On the one hand, we choose  $q_0$  so large, that for all  $q > q_0$  the differential effective cross sections  $d\Phi_n(q)$  for the excitations of the different levels  $n$  can be summed to  $d\Phi(q)$  by application of the completeness relation, i.e.,  $q_0 \gg a^2/K \times M/m$ . On the other hand, let  $q_0 \ll a$ , so that for all  $q > q_0$  the generalized transition probabilities  $\varphi_n(q)$  (cf. (33), (34)) may be replaced by the usual transition probabilities  $\varphi_n(0) = a^2 |x_{0n}|^2$ . Then according to (34), (17), and (38a)

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$$\left\{ \begin{aligned} \Phi' &= \sum_n \int_{q_{\min}}^{\infty} d\Phi_n(q) = \frac{8\pi}{K^2} \cdot \left( \frac{M}{m} z \right)^2 \cdot \sum_n \varphi_n(0) \int_{q_{\min}}^{\infty} \frac{dq}{q} \\ &= \frac{8\pi}{K^2} \cdot \left( \frac{M}{m} z \right)^2 \sum_n q_n \ln \frac{2q_n K m}{a^2 M \left( 1 - \frac{1}{n^2} \right)} \\ &= \frac{4\pi}{K^2} \left( \frac{M}{m} z \right)^2 \left[ \ln \frac{4q_{\max}^2 K^2 m^2}{a^4 M^2} - 2 \sum_{n=2}^{\infty} \varphi_n \ln \frac{n^2 - 1}{n^2} \right. \\ &\quad \left. - 2 \int_0^{\infty} dk \cdot \varphi_k \ln \left( 1 + \frac{k^2}{a^2} \right) \right]. \end{aligned} \right. \quad (52a)$$

Also, by (40), (19), and (37):

$$\begin{aligned} \Phi'' &= \int_{q_{\min}}^{q_{\max}} d\Phi_n(q) = \frac{8\pi n^2}{K^2} \left( \frac{M}{m} z \right)^2 \int_{q_{\min}}^{q_{\max}} \frac{dq}{q^2} \left( 1 - \frac{1}{\left( 1 + \frac{q^2}{4a^2} \right)^4} \right) \\ &= \frac{4\pi}{K^2} \left( \frac{M}{m} z \right)^2 \left[ \ln \frac{q^2}{4a^2 + q^2} + \frac{\frac{3}{4}}{1 + \frac{q^2}{4a^2}} + \frac{\frac{1}{4}}{\left( 1 + \frac{q^2}{4a^2} \right)^3} \right. \\ &\quad \left. + \frac{\frac{1}{12}}{\left( 1 + \frac{q^2}{4a^2} \right)^5} \right]_{q_{\min}}^{q_{\max}} \overset{q_{\max} \gg a}{}, \\ \Phi'' &= \frac{4\pi}{K^2} \left( \frac{M}{m} z \right)^2 \left( \ln \frac{4a^2}{q_{\max}^2} - \frac{13}{12} \right) \end{aligned} \quad (52b)$$

Except for magnitudes of the order of  $a^2/K^2$ :

$$\begin{aligned} \Phi &= \Phi' + \Phi'' = \frac{4\pi}{K^2} \left( \frac{M}{m} z \right)^2 \ln \frac{4m^2 K^4}{b M^3 a^2} \\ \ln b &= -\ln 4 + \frac{13}{12} + 2 \sum_{n=2}^{\infty} \varphi_n \ln \frac{n^2 - 1}{n^2} + 2 \int_0^{\infty} dk \varphi_k \ln \left( 1 + \frac{k^2}{a^2} \right). \\ \left\{ \begin{aligned} \ln b &= -\ln 4 + \frac{13}{12} - \frac{2}{3} \left[ \sum_{n=2}^{\infty} \frac{n^2(n-1)^2 n^{-3}}{(n+1)^{2n+6}} \ln \frac{n^2}{n^2-1} \right. \\ &\quad \left. - \int_0^{\infty} \frac{k dk a^6}{(a^2+k^2)^3} \cdot \frac{e^{-4\frac{a}{k} \arctan \frac{k}{a}}}{1-e^{-2\pi \frac{a}{k}}} \cdot \ln \left( 1 + \frac{k^2}{a^2} \right) \right]. \end{aligned} \right. \end{aligned} \quad (52c)$$

We find by numerical evaluation

$$\begin{aligned} b &= 0.638, \\ \Phi &= \frac{8\pi R h a^2 z^2}{m v^4} \ln \frac{2m v^4}{0.638 R h} = \frac{2\pi e^4 r^2}{R h \cdot m v^2} \ln \frac{2m v^2}{0.638 R h}. \end{aligned} \quad (53)$$

Multiplying by the number of atoms  $N$  per unit volume, we obtain the number  $N\Phi$  of inelastic collisions per centimeter path of the particle,

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i.e., the reciprocal mean free path. Essentially, this is inversely proportional to the square of the velocity of the particle and it also contains a logarithmic term. A corresponding logarithmic term also occurs in the number of the ions formed primarily from the particle per centimeter path, in contrast to Bohr's and Thomson's classical theory (cf. [18], [7, p. 606]). We obtain the number of primary ions

$$s_0 = N\Phi_i = N \int_0^{\infty} dk \int_{q_{\min}}^{q_{\max}} d\Phi_k(q)$$

most simply by subtracting the number of the discrete excitations

$$N\Phi_e = N \sum_{n=2}^{\infty} \int_{q_{\min}}^{q_{\max}} d\Phi_n(q)$$

from  $N\Phi$ . The result is

$$N\Phi_i = 0,715 \cdot \frac{2\pi e^4 z^2 N}{R h \cdot m v^3} \ln \frac{2m v^2}{1,79 R h} \quad (54a)$$

for the total number of excitations, and

$$N\Phi_e = s_0 = 0,285 \cdot \frac{2\pi e^4 z^2 N}{R h \cdot m v^3} \cdot \ln \frac{2m v^2}{0,018 R h} \quad (54b)$$

for the total number of ions formed per centimeter path. Likewise (integrating (40) over  $q$ ),

$$N\Phi_0 = \frac{4\pi N}{K^4} \left( \frac{M}{m} z \right)^4 \cdot \frac{7}{12} = 0,583 \cdot \frac{2\pi e^4 z^2 N}{R h \cdot m v^3} \quad (54c)$$

is the total number of elastic collisions per centimeter path; therefore, the latter does not contain any logarithmic term.

Now we compute quite analogously the total energy loss

$$E = \sum_n (E_n - E_0) \int_{q_{\min}}^{q_{\max}} d\Phi_n(q) \quad (55a)$$

of the particle flux per unit time. With respect to (45) and (46) we find, by analogy to (52a),

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$$\begin{aligned}
 E &= \sum_n \int_{q_{\min}}^q d\phi_n(q) (E_n - E_0) \\
 &= \frac{8\pi R h}{K^4} \left( \frac{M}{m} z \right)^2 \cdot \left[ \ln \frac{2q_u K m}{c^2 M} \right. \\
 &\quad - \sum_n q_n \left( 1 - \frac{1}{n^2} \right) \ln \frac{n^2 - 1}{n^2} - \int dk \varphi_k \\
 &\quad \left. \cdot \left( 1 + \frac{k^2}{n^2} \right) \ln \left( 1 + \frac{k^2}{n^2} \right) \right]. \tag{55b}
 \end{aligned}$$

Also, according to (47) and (20),

$$E' = \int_q^{q_{\max}} dE(q) = \frac{8\pi R h}{K^4} \left( \frac{M}{m} z \right)^2 \ln \frac{2K}{q_u} \frac{m}{M+m}. \tag{55c}$$

Therefore,

$$\begin{aligned}
 E &= \frac{8\pi R h}{K^4} \left( \frac{M}{m} z \right)^2 \ln \frac{4K^2}{c^2 n} \frac{m^2}{M(M+m)}, \\
 \ln c &= \frac{2^9}{3} \sum_{n=2}^{\infty} \frac{n^8 (n-1)^{2n-4}}{(n+1)^{2n+4}} \ln \frac{n^2 - 1}{n^2} \\
 &\quad + \frac{2^9}{3} \int_0^{\infty} dk \cdot k \cdot n^8 \cdot \frac{e^{-4 \frac{n}{k}} \operatorname{arctg} \frac{k}{n}}{1 - e^{-2n \frac{\pi}{k}}} \ln \left( 1 + \frac{k^2}{n^2} \right), \\
 c &= 1,105, \\
 E &= \frac{4\pi e^4 z^2}{m v^2} \ln \frac{(2) m v^2}{c R h}, \tag{55*}
 \end{aligned}$$

where the 2 in parentheses appears only for the collision of heavy particles, while it is disregarded in the case of electron collision.

The loss in kinetic energy per centimeter path is

$$-\frac{dT}{dx} = N E = \frac{4\pi e^4 z^2 N}{m v^2} \ln \frac{(2) m v^2}{c R h}. \tag{56}$$

This is almost exactly double the value derived by Henderson for the stopping cross section. Since Henderson's values are approximately half of the observed stopping cross section [9], our result agrees quite well with observation. Formula (56) differs from Bohr's formula for deceleration in that the argument of the logarithm contains  $v^2$  instead of  $v^3$ .

<sup>(\*)</sup> Read arctg as arc tangent.

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The mean energy loss of the particle per collision becomes

$$\bar{E} = \frac{E}{\phi} \approx 2Rh. \quad (57)$$

Since 28.5% of all collisions lead to ionization [(53) and (54b)], the energy consumption for each primarily formed ion is approximately  $2Rh/0.285$ ; which is seven times the ionization potential. This is the case with very high particle velocities; otherwise, the energy consumption per ion formed is somewhat smaller, since the logarithm in (54b) is appreciably larger than that in (55).

### III. MORE COMPLEX ATOMS

#### 11. f-Sum Rules

In this section we extend our results to more complex atoms, but, strictly speaking, we can do this for only a few points. In general we shall have to assume that the eigenfunctions of the atom may be represented as the sum of the products of the eigenfunctions of individual electrons, owing to which the simultaneous excitation of two electrons of the atom by the collision process is precluded from the very beginning. In numerical computation frequently we must go one step further - a precarious step - and replace the eigenfunctions of each electron by the hydrogen eigenfunctions of the corresponding quantum numbers. In all other cases we shall consider the eigenfunctions of an electron to be approximately the eigenfunctions computed by the Hartree method for a suitable potential field of the atom.

First we apply the generalized f-sum rule to atoms with several electrons; i.e., as in section 8, we are looking for the total energy transfer by collisions with a change in momentum between  $q$  and  $q + dq$ :

$$E(q) = \frac{8\pi}{K^2} \left( \frac{M}{m} z \right)^2 \frac{dq}{q} I(h) \sum_k f_{ek}(q). \quad (58)$$

$$f_{ek} = \frac{E_k - E_m}{K^2 h} \cdot \frac{a^2}{q^2} \cdot \left| \int \sum_j e^{iqx_j} \psi_m \overline{\psi_k} dx_j \right|^2. \quad (58a)$$

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Since no assumption had to be made about the potential  $V$  of Schrödinger's equation in deriving (45b),  $V$  in particular (as well as  $\Psi$ ) depend on more than three coordinates and (45b) applies directly to our case

$$\begin{cases} (E_k - E_m) \int \Psi_m \overline{\Psi}_k e^{iqx_j} d\tau \\ = R \hbar a^2 \left( -2iq \int \frac{\partial \Psi_m}{\partial x_j} \overline{\Psi}_k e^{iqx_j} d\tau + q^2 \int \Psi_m \overline{\Psi}_k e^{iqx_j} d\tau \right). \end{cases} \quad (58b)$$

Furthermore, from this we obtain

$$\begin{aligned} f &= \sum_k f_{mk} = \sum_k \left( -\frac{2i}{q} \int \sum_j e^{iqx_j} \cdot \frac{\partial \Psi_m}{\partial x_j} \overline{\Psi}_k d\tau \right. \\ &\quad \left. + \int \sum_j e^{iqx_j} \cdot \Psi_m \overline{\Psi}_k d\tau \right) \cdot \int \sum_l e^{-iqx_l} \cdot \overline{\Psi}_m \Psi_k d\tau, \\ f &= \sum_j \sum_l \left( -\frac{2i}{q} \int \frac{\partial \Psi_m}{\partial x_j} \overline{\Psi}_m e^{iq(x_j - x_l)} + \int \Psi_m \overline{\Psi}_m e^{iq(x_j - x_l)} \right). \end{aligned}$$

Since  $f$  is real by definition, it may easily be shown that in the first integral  $2\overline{\Psi}_m \frac{\partial \Psi_m}{\partial x_j}$  may be replaced by  $\frac{\partial |\Psi_m|^2}{\partial x_j}$ . Then, through partial integration we find that

$$-\frac{i}{q} \int \frac{\partial |\Psi_m|^2}{\partial x_j} e^{iq(x_j - x_l)} d\tau = \begin{cases} - \int |\Psi_m|^2 e^{iq(x_j - x_l)} & \text{for } j \neq l \\ 0 & \text{for } j = l \end{cases}$$

i.e.,

$$\begin{aligned} f &= \int \sum_j e^{iq(x_j - x_l)} |\Psi_m|^2 d\tau \\ f &= \sum_k f_{mk}(q) = Z. \end{aligned} \quad (59)$$

The sum of the generalized oscillator strengths (58a) for all transitions from one level of any atom is equal to the number  $Z$  of the electrons.

The transitions of a heavy atom from the ground state break down according to their transition frequency into different groups separated from each other to some extent, depending on whether an electron from the K, L, M, etc. shell is excited. It is questionable whether the oscillator strengths (58a) may also be summed by a simple process for each of these individual groups of transitions. Such a "partial f-sum rule" would be important for computing the total stopping cross section of an atom by integration over all possible collision vectors  $q$ . Since the lower

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integration boundary  $q_{\min}$  depends on the transferred excitation energy (17), it is advantageous to combine transitions with neighboring transition frequencies (excitation energies) before integration over  $q$ .

We can set up a partial f-sum rule if we assume, as indicated above, that the atomic eigenfunction may be represented as a sum of products of the eigenfunctions of individual electrons. Let us classify the latter by the principal quantum number  $n$  and the azimuthal quantum number  $\ell$ , and also a magnetic quantum number  $m$  (which is insignificant because of the azimuthal degeneracy); let  $Z_{nl}$  be the number of electrons in an atom in the ground state in the  $(nl)$ -shell, let  $\vec{Z}_{nl}$  and  $Z_{nl}$  be the numbers of  $(nl)$ -electrons of the individual spin directions  $(\vec{Z}_{nl} = \vec{Z}_{nl} + \vec{Z}_{nl})$ , and let  $g_{nl} = 2\ell + 1$  be the "weight" of the electron state  $(nl)$ . Then it may easily be shown that the square of the matrix element for the transition of an electron from the  $nl$ -shell to  $n'l'$  is given by

$$\left\{ |\epsilon_{nl,n'l'}(q)|^2 = \left[ \vec{Z}_{nl} \left( 1 - \frac{\vec{Z}_{n'l'}}{g_{n'l'}} \right) + \vec{Z}_{nl} \left( 1 - \frac{\vec{Z}_{n'l'}}{g_{n'l'}} \right) \right] |\epsilon_{nl,n'l'}(q)|^2; \quad (60) \right.$$

$$|\epsilon_{nl,n'l'}(q)|^2 = \frac{1}{g_{nl}} \cdot \sum_{m=-l}^{+l} | \int \psi_{nlm} \bar{\psi}_{n'l'm} e^{iqx} d\tau |^2 \quad (60a)$$

is the square of the matrix element for the case where one electron is in the  $(nl)$ -state and the  $(n'l')$ -state is unoccupied, i.e., for the case which always applies for the hydrogen atom. <sup>\*\*</sup>) The factor which occurs

<sup>\*</sup>) In the case of the ground state, these numbers may be given individually. Since the ground term is a term of the highest multiplicity, when  $\rightarrow$  gives the direction of the total spin,  $\vec{Z}_{nl}$  must be as large as possible, i.e.,  $\vec{Z}_{nl} = Z_{nl}$  when  $Z_{nl} < g_{nl}$ , and  $\vec{Z}_{nl} = g_{nl}$  when  $Z_{nl} > g_{nl}$ .

<sup>\*\*</sup>) As in (60a), averaging over  $m$  should also be done for the hydrogen atom. If we do not combine all transitions from the  $nl$ -shell, but consider transitions from each individual quantum cell (characterized by  $n$ ,  $\ell$ ,  $m$ , and the spin direction) individually, the matrix element becomes even simpler, viz.,  $\epsilon_{nlm, n'l'm} = \int e^{iqx} \psi_{nlm} \bar{\psi}_{n'l'm}$ . (60b)

when  $lm$  is occupied and  $n'l'm$  empty, but it is zero when  $nlm$  is unoccupied or  $n'l'm$  is occupied (or both), i.e., it is as though only the one "jumping" electron were present in the atom. However, the distribution of electrons to individual places with a different  $m$  within an  $(nl)$ -level cannot be given and, therefore, averaging must be done over all electron position distributions possible with the given total number of electrons in the  $(nl)$ -shell. This averaging yields (60, 60a).

both in (60a) and (60) and depends both on the number of electrons in the initial level and the number of vacant positions in the final level is quite evident from the viewpoint of the Pauli principle.

From (60) we may compute the sum of the oscillator strengths for all transitions in which an electron from the  $(nl)$ -shell is excited:

$$\left\{ \begin{array}{l} f_{nl} = \sum_{n'l'} f_{nl,n'l'} = \frac{\alpha^2}{q^2 R h} \sum_{n'l'} (E_{n'l'} - E_{nl}) |\epsilon_{nl,n'l'}(q)|^2 \\ = \frac{\alpha^2}{q^2 R h} \left( Z_{nl} \sum_{n'l'} (E_{n'l'} - E_{nl}) |\epsilon_{nl,n'l'}^1(q)|^2 \right. \\ \left. - \sum_{n'l'} \frac{\vec{Z}_{nl} \vec{Z}_{n'l'} + \vec{Z}_{nl} \vec{Z}_{n'l'}}{g_{n'l'}} (E_{n'l'} - E_{nl}) |\epsilon_{nl,n'l'}^1(q)|^2 \right). \end{array} \right. \quad (61a)$$

The first summand may be computed in exact analogy to the derivation of the f-sum rule for hydrogen (section 8) and is found to be  $Z_{nl}$ ; furthermore, if

$$\left\{ \begin{array}{l} f_{nl,n'l'}^1 = (E_{n'l'} - E_{nl}) \frac{\alpha^2}{q^2 R h} |\epsilon_{nl,n'l'}^1(q)|^2 \\ = \frac{\alpha^2}{q^2 R h} (E_{n'l'} - E_{nl}) \\ \cdot \frac{1}{g_{nl}} \sum_m \left| \int \psi_{nlm} \bar{\psi}_{n'l'm} e^{iqz} dz \right|^2, \end{array} \right. \quad (61)$$

we will have

$$\left\{ \begin{array}{l} f_{nl} = Z_{nl} - \sum_{n'l'} \frac{\vec{Z}_{nl} \vec{Z}_{n'l'} + \vec{Z}_{nl} \vec{Z}_{n'l'}}{g_{n'l'}} \cdot f_{nl,n'l'}^1 \\ = \sum_{n'l'} f_{nl,n'l'}^1 \zeta. \end{array} \right. \quad (62)$$

The sum of the oscillator strengths of all transitions in which an electron from the  $(nl)$ -shell is excited is equal to the number  $Z_{nl}$  of the electrons in this shell, less the oscillator strengths of the transitions from the  $nl$ -state forbidden by the Pauli principle. If all  $n''l''$ -shells are occupied and all others are vacant,  $\vec{Z}_{n''l''} = \vec{Z}_{n''l''} = g_{n''l''}$  and

$$f_{nl} = Z_{nl} \left( 1 - \sum_{n'l'} f_{nl,n'l'}^1 \right). \quad (62a)$$

The partial sum  $f_{nl}$  of the oscillator strengths is smaller or greater than the number of electrons  $Z_{nl}$  in the  $(nl)$ -shell, depending on whether

$(nl)$  is an inner or an outer shell of the atom. If  $(nl)$  is an inner shell, the oscillator strengths  $f_{nl}^l$ ,  $n'l'$  are positive for all transitions forbidden by the Pauli principle because  $E_{n'l'} > E_{nl}$ , and the reverse is true for outer shells. \*) If we sum the oscillator strengths for all possible transitions of the atom, we obtain

$$j = \sum_{nl} j_{nl} = \sum_{nl} Z_{nl} - \frac{e^2}{q^2 h \hbar} \sum_{nl} \sum_{n'l'} \frac{\vec{Z}_{nl} \vec{Z}_{n'l'} + \vec{Z}_{nl} \vec{Z}_{n'l'}}{g_{nl} g_{n'l'}} \\ \cdot (E_{n'l'} - E_{nl}) \sum_m \left| \int e^{iqx} \psi_{nlm} \bar{\psi}_{n'l'm} d\tau \right|^2 = Z.$$

The deviations of the partial sums  $f_{nl}$  from the numbers of electrons  $Z_{nl}$  in the individual shells necessarily become more prominent when all oscillator strengths of the atom are summed.

We give the oscillator sums  $f_{nl}/Z_{nl}$  for the individual  $(nl)$ -shell of various atoms \*\*) in table 2 to establish a criterion for the order of magnitude of the expected effects. They are greatest (up to 1.7) for outer shells of high azimuthal quantum numbers, since the transition probabilities in the hydrogen atom are greatest for transitions from  $(n-1, l = n-2)$  to  $(n, l = n-1)$  and because the oscillator sum  $f_{n, n-1}$  increases by the oscillator strength of this transition when it is forbidden. On the other hand, outer  $(ns)$ -shells have oscillator sums that are not appreciably greater than 1, because the transition probabilities  $n-1, l \rightarrow n, 0$  are very small, as is generally true of the probabilities of all transitions in which the principal and secondary quantum numbers vary inversely with respect to one another. Oscillator sums for inner shells in heavy atoms decrease to approximately 0.3 to 0.4 per

\*) I was reading the proofs of the present paper when I learned that this law had already been discovered by R. de.L. Kronig and H. A. Kramers [19]. This law has also been confirmed experimentally: Dispersion and absorption measurements in the x-ray region show the sum of the oscillator strengths of the K-series to be considerably smaller than 2 (see the literature cited in [19]).

\*\*) The number of forbidden transitions increases with the atomic number, and the oscillator sums change accordingly. In computing the oscillator strengths (61), we introduced hydrogen eigenfunctions for the  $\psi_{nlm}$ ; the transition probabilities were taken from the numerical tables of Kupper [20].

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electron,<sup>\*)</sup> then a K-electron, for example, may be raised practically only to a state of the continuous spectrum and not to one of the discrete spectrum; thus, practically the only remaining oscillator strengths are those of the transitions to the continuous spectrum.

Table 2  
Oscillator sums for several levels in various atoms

	Be	B	C	N	O	F	Ne	Na	Mg
1s . . .	1,000	,931	,861	,792	,723	,653	,584	,584	,584
2s . . .	1,000	1,000	1	1	1	1	1	1	1
2p . . .	—	1,136	1,136	1,136	1,136	1,136	1,136	1,120	1,122
3s . . .	—	—	—	—	—	—	1,040	1,040	—

	Ne	Ar	Cu	Kr	Ag	Xe	Au	Em
1s . . .	,554	,505	,503	,476	,476	,463	,463	,455
2s . . .	1,000	,565	,565	,462	,462	,420	,420	,398
2p . . .	1,136	1,122	,426	,423	,301	,300	,256	,256
3s . . .	—	1,040	1,040	,566	,566	,446	,446	,394
3p . . .	—	1,171	1,171	1,138	,533	,528	,387	,387
3d . . .	—	—	1,418	1,407	1,407	1,403	,408	,408
4s . . .	—	—	—	1,103	1,103	,360	,322	,422
4p . . .	—	—	—	1,220	1,220	1,070	,450	,450
4d . . .	—	—	—	—	1,437	1,464	1,464	1,456
4f . . .	—	—	—	—	—	—	1,712	1,712

## 12. Deceleration

We compute the total energy transferred from the particle flux to the atom per unit time

$$E = \frac{8\pi a^3}{K^2} \left( \frac{M}{m} z \right)^2 \sum_k (E_k - E_0) \int_{q_{\min}}^{q_{\max}} \frac{dq}{q^2} |\epsilon_{0k}(q)|^2 \quad (63)$$

in a manner quite similar to that used in section 10 for the hydrogen atom: We divide the integration region  $q_{\min}$  to  $q_{\max}$  by a point of intersection into two parts; in the first part ( $q_{\min}$  to the point of intersection) we first integrate over  $q$  for each transition separately and only then sum over all possible transitions  $k$ . Starting from the point of intersection, we use the partial f-sum rule of the preceding section to combine all those transitions in which an electron of the  $(nl)$ -shell is excited, and only then integrate over  $q$ . We do not choose the point

<sup>\*)</sup> If we do not introduce hydrogen eigenfunctions but consider the screening, the forbidden transitions become weaker and all oscillator sums approach unity (cf. [19]).

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of intersection itself for all transitions of the atom equal to ( $q_0$ ) as in section 10, but only for those transitions in which an ( $n\ell$ )-electron is excited ( $q_{n\ell}$ ); the  $q_{n\ell}$ 's may be different for various  $n\ell$ -shells. We determine each point of intersection  $q_{n\ell}$  such that practically all excitations of the ( $n\ell$ )-electron are possible, from the standpoint of energy, for all  $q > q_{n\ell}$ ; thus,

$$q_{n\ell} \gg \frac{a_{n\ell}^2 M}{2 K m},$$

where

$$a_{n\ell}^2 = - \frac{8\pi^2 m}{h^4} E_{n\ell}$$

and  $-E_{n\ell}$  is the ionization potential of the  $n\ell$ -shell.\*). On the other hand, the transition probabilities for all  $q < q_{n\ell}$  should be indicated by their value at  $q = 0$ , viz., by the elements of the coordinate matrix, i.e.,  $q_{n\ell} \ll a_{n\ell}$  (cf. the corresponding choice of the point of intersection  $q_0$  for the hydrogen atom). Then (cf. (55b), (55c)) in view of (61a) and (62), we will have

$$\left| \begin{aligned} E &= \frac{8\pi R h}{K^4} \left( \frac{M}{m} z \right)^2 \sum_{n\ell} \left( \sum_{n'\ell'} f_{n\ell, n'\ell'}(0) \ln \frac{2q_{n\ell} K m}{(a_{n\ell}^2 - a_{n'\ell'}^2) M} \right. \\ &\quad \left. + \int_{q_{n\ell}}^{q_{\max}} f_{n\ell}(q) \frac{dq}{q} \right) \\ &= \frac{8\pi R h}{K^4} \left( \frac{M}{m} z \right)^2 \sum_{n\ell} \left( f_{n\ell}(0) \ln \frac{2q_{n\ell} K m}{a_{n\ell}^2 \cdot M} \right. \\ &\quad \left. + \sum_{n'\ell'} f_{n\ell, n'\ell'}(0) \ln \frac{-E_{n\ell}}{E_{n'\ell'} - E_{n\ell}} \right. \\ &\quad \left. + Z_{n\ell} \ln \frac{2 K m}{q_{n\ell} (M + m)} - \sum_{n'\ell'} \int_{q_{n\ell}}^{q_{\max}} f_{n\ell, n'\ell'}(q) \frac{dq}{q} \right. \\ &\quad \left. - \frac{\overrightarrow{Z}_{n\ell} \overrightarrow{Z}_{n'\ell'} + \overrightarrow{Z}_{n\ell} \overleftarrow{Z}_{n'\ell'}}{g_{n'\ell'}} \right). \end{aligned} \right. \quad (63a)$$

Here, due to definition (61a) of  $f_{n\ell, n'\ell'}$ , the sum over  $n'\ell'$  applies to all vacant electron states, while the sum over  $n'\ell'$  applies to the occupied states. Since, according to (61),

\*).  $a_{n\ell}$  is of the type of reciprocal lengths  $a_n$  in section 4 that relate to the state of the atom (electron), not of the type of the  $a_{0n}$ 's in section 4 that relate to transitions.

$$g_{nl} f_{nl, n'l'}^1 = - g_{n'l'} f_{n'l', nl}^1, \quad (63b)$$

by combining two terms each in the sum over  $n'l'$  which correspond to the transition  $nl \rightarrow n'l'$  and to the inverse transition, we get

$$\left\{ \begin{aligned} & - \int_{q_{nl}}^{q_{max}} \frac{f_{nl, n'l'}^1(q)}{g_{n'l'}} \frac{dq}{q} - \int_{q_{nl}}^{q_{max}} \frac{f_{n'l', nl}^1(q)}{g_{nl}} \frac{dq}{q} \\ & = \int_{q_{nl}}^{q_{nl}} \frac{f_{nl, n'l'}^1(q)}{g_{n'l'}} \frac{dq}{q} \quad (63c) \\ & \approx \int_{q_{nl}}^{q_{nl}} \frac{f_{nl, n'l'}^1(0)}{g_{n'l'}} \frac{dq}{q} = - \frac{f_{nl, n'l'}^1(0)}{g_{n'l'}} \ln \frac{2Km}{q_{nl}(M+m)} \\ & - \frac{f_{n'l', nl}^1(0)}{g_{nl}} \ln \frac{2Km}{q_{nl}(M+m)}. \end{aligned} \right.$$

(The substitution of  $f_{nl, n'l'}^1(0)$  for  $f_{nl, n'l'}^1(q)$  is permissible for  $q < q_{nl}$  or  $q_{n'l'}$ , because the points of intersection  $q_{nl}$  are chosen such that the generalized oscillator strengths there do not yet deviate essentially from their value at  $q = 0$  (i.e., from the oscillator strengths defined in the usual manner)). Therefore, in view of (62)

$$\left\{ \begin{aligned} E &= \frac{8\pi R \hbar}{K^4} \left( \frac{M}{m} z \right)^2 \sum_{nl} f_{nl} \\ & \cdot \left( \ln \frac{4K}{\sigma_{nl} M(M+m)} + \frac{1}{f_{nl}} \sum_{n'l'} \zeta f_{nl, n'l'}^1 \ln \frac{-E_{nl}}{E_{n'l'} - E_{nl}} \right), \end{aligned} \right. \quad (63d)$$

where the oscillator strengths  $f_{nl, n'l'}^1$  and the partial oscillator sums  $f_{nl}$  mean the values of these quantities at  $q = 0$ . In order to write (63d) more conveniently, we define the mean excitation energy of the ( $nl$ )-shell:

$$\left\{ \begin{aligned} f_{nl} \ln A_{nl} &= f_{nl} \ln (-E_{nl}) \\ & + \sum_{n'l'} f_{nl, n'l'}^1 \left( Z_{nl} - \frac{\overset{\leftarrow}{Z}_{nl} \overset{\leftarrow}{Z}_{n'l'} + \overset{\rightarrow}{Z}_{nl} \overset{\rightarrow}{Z}_{n'l'}}{g_{n'l'}} \right) \cdot \ln \frac{E_{n'l'} - E_{nl}}{-E_{nl}}. \end{aligned} \right. \quad (64)$$

For an outer shell, the mean excitation energy is generally somewhat lower than the ionization potential  $-E_{nl}$  of the shell. The transitions to the next higher discrete levels (especially to  $n' = n + 1$ ,  $l' = l + 1$ ) have the highest oscillator strengths  $f_{nl, n'l'}^1$ ; however, for these

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transitions  $E_{n'l'} - E_{nl} < 0$ , i.e.,  $\ln \frac{E_{n'l'} - E_{nl}}{-E_{nl}} < 0$ , therefore, if the level  $n'l'$  is vacant, these transitions yield a large negative contribution to the sum in (64), in comparison to which the positive contribution of the transitions to the continuous spectrum is negligible. \*) In any case, the mean excitation energy is greater (even for outer shells) than the energy for the initial excitation (excitation of the "resonance line"), as may easily be seen from (64). We may safely assume that the mean excitation energy is greater than that of the excitation potential of the resonance line by a factor of 1.2 to 1.5; at any rate, rough computations using hydrogen eigenfunctions give this result. \*\*)

For inner shells, ionization is practically the only effect possible; the mean excitation energy is approximately 30 to 60% higher than the ionization potential.

If we use the mean excitation energy, (63d) becomes

$$E = \frac{4\pi e^4 z^2}{m v^2} \sum_{nl} f_{nl} \ln \frac{(2) m v^2}{A_{nl}}. \quad (65)$$

The 2 in parentheses in the logarithm stands for the case of collision of heavy particles only (see (55)) and does not apply to electron collision.

Hence, the total energy loss of the particle per centimeter path

$$-\frac{d T}{d x} = N E = \frac{4\pi e^4 z^2 N}{m v^2} \sum_{nl} f_{nl} \ln \frac{(2) m v^2}{A_{nl}} \quad (66)$$

\*) The case where ls is the outermost shell (H, He) is an exception. Here, the excitation energy for discrete transitions differs very little from the ionization potential (by 25% at most), while it lies considerably above the ionization potential, on the average, for the high energy transitions into the continuous spectrum; therefore, the continuous transitions here yield the greater contribution to the sum in (64) and the mean excitation energy becomes somewhat greater (10%) than the ionization potential (cf. section 10, formula (55)).

\*\*) The stopping cross section is not sensitive to errors in the mean excitation energy.

is composed of the energy losses to individual shells. The energy loss to each shell is not proportional to the number of electrons in the shell, but rather to the oscillator sum  $f_{nl}$  which differs somewhat from it (cf. table 2); in addition, the stopping cross section (energy loss) for every shell contains a logarithmic term, as in classical theories. Both the logarithmic term and the replacement of the number of electrons  $Z_{nl}$  by the oscillator sum  $f_{nl}$  cause the outer shells to have a greater stopping cross section than the inner ones; however, the stopping cross sections of the outer and inner shells relative to the fast particles do not differ by orders of magnitude, but at most by a factor of about 5.

### 13. Comparison of the Stopping Cross Section with Earlier Theories and with Observation

Our formula for the stopping cross section

$$-\frac{dT}{dx} = -M_1 v \frac{dv}{dx} = \frac{4\pi e^4 z^2 N}{m v^2} \sum_{nl} f_{nl} \ln \frac{2m r^2}{A_{nl}} \quad (66a)$$

is most like that of Henderson [8]. This is quite natural, since Henderson's theory goes beyond all previous ones in the use of quantum-theoretical propositions. Equation (66) differs from Henderson's formula chiefly by a factor of 2; this factor makes our formula agree well with observation, since Fowler [9] has shown that the stopping cross section computed according to Henderson turns out to be about 50% too low (cf. below). Henderson's idea is to compute the transfer of energy from the particle to an electron of the atom by classical means but to regard only collisions with a transfer of energy greater than the ionization potential as admissible by quantum theory; this idea has a basis in fact. According to wave mechanics, the f-sum rule for the transfer of energy to an ( $nl$ )-electron in collisions in which the particle momentum changes by  $M(v - v')$  between  $\frac{h}{2\pi}q$  and  $\frac{h}{2\pi}(q + dq)$  gives us \*)

$$E(q) = \frac{4\pi e^4 z^2}{m v^2} \frac{dq}{q} \cdot \frac{f_{nl}(q)}{Z_{nl}}. \quad (67)$$

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\*) Provided that  $q$  is large enough to permit all transitions of the ( $nl$ )-electron.

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Moreover, classically each of these collisions involves an energy loss \*)

$$\left\{ \begin{array}{l} Q = \frac{M_1}{2} (v^2 - v'^2) = \frac{m M_1^2}{2(m + M_1)} |v - v'|^2 \\ = \frac{m M_1^2}{M^2(m + M_1)^2} \cdot \frac{\hbar^2}{8\pi^2} Q^2 = \text{const} \cdot Q^2 \end{array} \right. \quad (67a)$$

and, except for the replacement of the oscillator sums  $f_{nl}$  by the electron numbers  $Z_{nl}$ , we get the same formula classically as we do wave mechanically (cf. [9, p. 526]) for the energy loss during these collisions.  $W(Q)$  is the probability of the collisions.

$$E(Q) = Q \cdot W(Q) = \frac{2\pi e^4 z^2}{mc^4} \frac{dQ}{Q}. \quad (67b)$$

Computing the smallest "classically transferable energy" from the minimum change of momentum permitted by quantum mechanics,

$$q_{\min} \approx \frac{Ma_{nl}^2}{2mK}$$

(cf. (17)), we obtain

$$Q_{\min} \approx \frac{m}{M^2} \frac{\hbar^2}{8\pi^2} q_{\min}^2 = \frac{m}{4M} \cdot \frac{E_{nl}^2}{T_e}, \quad (67c)$$

Thus, contrary to Henderson's hypothesis, the minimum transferable energy is very much lower than the ionization potential, consequently our stopping cross section is twice as large as Henderson's. \*\*)

Curiously, Gaunt [10] obtains a result completely different from ours. Treating the colliding particle as a corpuscle and the atom wave mechanically, for hydrogen he again obtains Bohr's formula for deceleration

\*) Classically, the inelastic collisions are treated as elastic collisions between the particle and an atomic electron. Thus, from our formula (21) for the total energy lost by a particle during collision, only the first (classical) term appears on the right side; however, in this term we have to substitute  $m$  for  $M_2$  (mass of the struck particle) and  $M_1 m / m + M_1$  for  $M$  (effective mass of the colliding particle).

\*\*) Besides, integration of the classical formula from  $Q_{\min}$  to  $Q_{\max} = m/2 v^2$  gives a correct result only for electrons. For  $\alpha$ -particles, the classical hypothesis of "collision with the atomic electron according to the momentum principle" is too crude for small deflections - in the logarithm one obtains one factor  $M/m$  too many.

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$$-\frac{dT}{dx} = \frac{4\pi e^4 z^2 N}{m v^4} \ln \frac{m v^4}{0.53 \cdot 2\pi \cdot R \cdot e^2 z} \quad (68)$$

which, with respect to the argument in the logarithm, differs from our formula by the factor \*)

$$\frac{1.12 \cdot h v}{2\pi e^2 z} \quad (68a)$$

Perhaps the reason is that Gaunt disregards the fate of the particle during the collision and thus includes collisions in which the energy balance is not fulfilled at all, i.e., in which the classically-treated particle loses less energy than is gained (quantum mechanically) by the atom. Furthermore, he complicates his calculation needlessly by mixing classical and quantum mechanical methods.

To compare our theory with experiment, like Fowler ([9]) we do not compute the total range, which would naturally be given by integral logarithm of the initial velocity of the particle, but rather the path length  $X$  needed to decelerate an  $\alpha$ -particle of radium C' from the initial velocity  $v = 1.922 \times 10^9 \text{ cm sec}^{-1}$  to 90% of this value. Then, in the logarithm on the right side of (66) we can replace  $v^2$  by a mean value. We express  $m/2 v^2$  in electron volts - it is the energy of an electron having the same velocity as the  $\alpha$ -particle. According to Fowler,

$$\frac{m}{2} v^2 = W = 940 \text{ volts}$$

and we obtain

$$\frac{v_0^4 - v^4}{X} = \frac{16\pi e^4 z^2 N}{m M_1} \sum_{n=1} f_{n1} \ln \frac{4W}{A_{n1}} \quad (69)$$

and, by substituting constants (for  $15^\circ\text{C}$ ),

$$\left\{ \begin{array}{l} B = \sum_{n=1} f_{n1} \cdot 10 \log \frac{4W}{A_{n1}} = \\ = \frac{0.4343 \cdot (1.922)^4 \cdot 10^{30} \cdot (1-0.9)^4 \cdot 4 \cdot 1830 \cdot 0.81 \cdot 10^{-31} \cdot 2.21 \cdot 10^4 \cdot 235}{16 \cdot 3.14 \cdot (4.77)^4 \cdot 10^{-40} \cdot 2^2 \cdot 6.1 \cdot 10^{23} \cdot 273 \cdot X} = .5 \end{array} \right. \quad (69a)$$

\*) Although for normal  $\alpha$ -particles ( $v = 1$  to  $2 \times 10^9 \text{ cm sec}^{-1}$ ) the factor is of the order of magnitude of 2 to 4 (i.e., since it is contained in the logarithm, it is of but little consequence), the form of the law is nevertheless considerably changed.

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Table 3 gives the experimental and the theoretical values of the stopping cross section  $B$  for several elements. \*) The oscillator sums  $f_{nl}$  are taken from table 2, i.e., computed on the basis of hydrogen eigenfunctions; for the mean excitation potentials we substituted the resonance potential, increased by a factor of 1.5, in outer shells and the ionization potential, increased by a factor of 1.5, in inner shells; we used the values given by Fowler in [9] for both the excitation and the ionization potentials.

Table 3  
Stopping Cross Sections

$Z$	Substance	$B_{\text{obs.}}$	$B_{\text{cal.}}$	Error %
1	$\frac{1}{2} \text{H}_2$	2,67	2,42	- 9
2	He	5,03	4,24	- 15
7	$\frac{1}{2} \text{N}_2$	—	13,4	—
7,2	$\frac{1}{2} \text{Luft}$	12,0	13,8	+ 15
8	$\frac{1}{2} \text{O}_2$	13,3	15,4	+ 15
10	Ne	—	18,4	—
13	Al	18,7	20,7	+ 11
18	A	21	27,1	+ 13
29	Cu	31,7	49,9	+ 57
79	Au	48,4	95,6	+ 07

For  $\text{H}_2$ , He, air,  $\text{O}_2$ , Al, and Ar, our formula is in very good agreement with experiment; in the case of heavier elements, it systematically yields excessive values for the stopping cross section. The partial oscillator sums for all transitions proceeding from one level would probably be considerably closer to 1 if, instead of the hydrogen eigenfunctions, we used eigenfunctions that are more suitable for computing oscillator strengths, e.g., Hartree's eigenfunctions. This would reduce the stopping cross section of the outer shells as well as the total stopping cross section. The error that may be caused by incorrect values for the mean excitation potential can be smaller. Errors

\*) Although the expression  $\frac{v_0^4 - v^4}{X}$  is generally designated as the stopping cross section, it is cumbersome owing to its magnitude. Our stopping cross section differs from Fowler's S-value by a factor of  $0.217 = \frac{1}{Z} \times 10 \log e$ .

are more likely to arise from our use of formulas taken from Born's collision theory for the middle shells as well, although there our hypothesis (ionization potential small relative to  $\frac{m}{2} v^2$ ) no longer holds. At any rate, it is gratifying that the agreement with observation is best in the case of light atoms, for which our hypotheses are most likely to be correct.

On the other hand, our formula does not offer a basis for deriving a general law of the dependence of the stopping cross section on the atomic number. We can only observe from the increasing number of sum terms in formula (66) that the stopping cross section grows with increasing atomic number, but not as rapidly as  $Z$  (since the individual terms (the logarithms) are very much smaller for inner than for outer shells, and since in more complex atoms it is mainly new inner shells that are added). A particularly large stopping cross section should be found in all atoms having many electrons in the outer shells, i.e., in noble gases (in agreement with observation) as well as in elements with closed 18-electron shells, e.g., Cu, Ag, and Au (contrary to observation).

The particle's energy loss per centimeter of path is less dependent on velocity for heavy decelerating atoms than for light atoms, for if we rewrite (66) as

$$-\frac{dT}{dx} = \frac{4\pi e^4 z^2}{\mu v^2} Z \ln \frac{2mr^2}{E}, \quad (70)$$

the mean excitation energy of the atom  $E$  is defined by \*)

$$Z \ln E = \sum_{nl} f_{nl} \ln A_{nl} \quad (70a)$$

and it increases with the number of inner shells having a high excitation potential. Hence, in heavy atoms the mean excitation energy  $E$  is more nearly equal to the energy  $W = \frac{m}{2} v^2$ , so that if the velocities

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\*) On the right side, only the terms  $A_{nl} < \frac{m}{2} v^2$  are to be computed; correspondingly,  $Z$  should be replaced by  $\sum f_{nl}$  for all those  $nl$ -shells for which this inequality holds.

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$v$  are not excessively large, the logarithm in (70) becomes relatively small; the change of the logarithm with velocity, however, is always

$$\frac{d}{dv} \ln \frac{mv^2}{E} = \frac{2}{v}$$

i.e., independent of the decelerating atom, and thus the relative change is greater with heavy atoms than with light atoms. Therefore, owing to the factor  $1/v^2$ , the decrease of the stopping cross section at a reasonable particle velocity  $v$  is partially balanced by an increase in the logarithm. The increase is relatively larger in the case of deceleration by heavy atoms than by light atoms; therefore, in heavy atoms the resulting decrease in the stopping cross section with increasing velocity is smoother and the range of the particle varies with a lower power of the velocity than in the case of light atoms, as indicated by observation.\*<sup>1</sup>) For very large particle velocities (fast electrons), the change of the logarithm in (70) with velocity becomes insignificant, the energy loss becomes proportional to  $1/v^2$ , and the range proportional to  $v^4$ ; this is the Thomson-Whiddington law [22, 23]. If we compute the constant of this law\*\*<sup>2</sup>)

$$\frac{\rho Z}{A} \cdot b = \frac{v_0^4 - v^4}{x} = \frac{16\pi e^4 L}{m^4} \cdot \frac{\rho Z}{A} \cdot \ln \frac{mv^2}{E} \quad (70b)$$

e.g., for the velocity  $10^{10} \text{ cm sec}^{-1} = 30,000 \text{ volts}$ , we obtain for air (mean excitation energy  $E = 35 \text{ volts}$ )  $b = 14 \times 10^{42}$  and for Cu ( $E \approx 80 \text{ volts}$ )  $b = 12.5 \times 10^{42}$ , which in both cases is somewhat higher than the experimental results ( $10$  to  $11 \times 10^{42}$ ) [24, 25]. The constant  $b$  should increase slightly with increasing velocity (e.g., by  $1 \times 10^{42}$  if the kinetic energy of the electron is doubled), but the experiments do not allow a decision on this.

\*<sup>1</sup>) Cf. [21]. The principle that the range is proportional to  $v^3$  (i.e., that the stopping cross section is proportional to  $1/v$ ) is satisfied well in the case of air, but this must be considered a coincidence.

\*<sup>2</sup>)  $L$  is the Loschmidt number,  $\rho$  is the density, and  $A$  is the atomic weight of the decelerating substance.

#### 14. Excitation of Optical Levels

According to (60), the differential effective cross section for the excitation of an electron to the  $n'l'$ -state is

$$d\Phi_{n'l'}^{n'l}(q) = \frac{8\pi a^2}{q^2 K^2} dq \left( \frac{M}{m} z \right)^2 \cdot \zeta \cdot |\epsilon_{nl, n'l'}^1(q)|^2 \quad (71)$$

where  $|\epsilon_{nl, n'l'}^1(q)|^2$  is given by (60a) and  $\zeta$  is defined in (62). The total probability (the integral excitation cross section) for this transition is obtained by integration over  $q$ . When  $n'l'$  is a discrete atomic state, the region  $q \gg a_{nl}$  is not involved because its matrix elements for discrete transitions almost disappear, owing to interference by the contributions of the individual volume elements to  $\int \psi_{nl} \bar{\psi}_{n'l'} e^{iqx} d\tau$  (see sections 6 and 9); the factor  $1/q^3$  is also in (71). Moreover, since

$$\left\{ \begin{array}{l} |\epsilon_{nl, n'l'}^1(q)|^2 = \frac{1}{g_{nl}} \sum_n |f c' \epsilon^* \psi_{nlm} \bar{\psi}_{n'l'm} d\tau|^2 \\ = \frac{q^2}{g_{nl}} \sum_n |\int \psi_{nlm} \bar{\psi}_{n'l'm} x d\tau|^2 = q^2 |x_{nl, n'l'}|^2 \end{array} \right. \quad (71a)$$

is  $q^2$ -times the optical transition probability for  $q \ll a_{nl}$ , it follows by approximation that\*)

$$\left\{ \begin{array}{l} \Phi_{n'l'}^{n'l} \approx \frac{8\pi a^2}{K^2} \left( \frac{M}{m} z \right)^2 \cdot \zeta \cdot |x_{nl, n'l'}|^2 \int_{q_{min}}^{q_{max}} \frac{dq}{q} \\ \Phi_{n'l'}^{n'l} \approx \frac{8\pi R \hbar}{m v^2} z^2 |x_{nl, n'l'}|^2 \\ \left( Z_{nl} - \frac{\vec{Z}_{nl} \cdot \vec{Z}_{n'l'} + \vec{Z}_{nl} \cdot \vec{Z}_{n'l'}}{g_{nl} v} \right) \ln \frac{2 m v^2}{E_{n'l'} - E_{nl}} \end{array} \right. \quad (72)$$

i.e., the excitation cross section for a collision of fast electrons or  $\alpha$ -particles is approximately proportional to the optical transition probability, and, furthermore, is inversely proportional to the square of the velocity of the electron and proportional to the logarithm of the quotient of the kinetic energy of the electron over the excitation potential. Hence, strong optical transitions are excited with particular intensity, especially the transition corresponding to the emission of the "resonance line" (cf., e.g., [26]).

\*) That is, except for one factor of the order of 1.

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Of course, excitation of transitions without an optical transition probability, i.e., without a dipole moment, is not entirely forbidden; for the excitation cross section of a transition with a quadrupole moment, we get, e.g.,

$$\sum_n | \int e^{i\epsilon_{n'l}} \psi_{nlm} \bar{\psi}_{n'l'm'} d\tau |^2 = \frac{q^4}{4} \sum_n | \int x^2 \psi_{nlm} \bar{\psi}_{n'l'm'} d\tau |^2 \\ = \frac{q^4}{4} | x^2_{nlm, n'l'm'} |^2$$

for  $q \ll a_{nl'}$ , while interference of the contributions of the individual volume components causes the integral on the left to approach zero again at large values of  $q$ . Thus, for such transitions

$$\left\{ \begin{array}{l} \Phi_{n'l'}^{(1)} \approx \frac{2\pi n^2}{K^2} \left(\frac{M}{m}\right)^2 |x^2_{nlm, n'l'm'}|^2 \zeta \int_{r_{nlm}}^{r_{n'l'm'}} q dq \\ = \frac{2\pi R h c^2}{m v^2} |x^2_{nlm, n'l'm'}|^2 a_{nl}^2 \zeta \end{array} \right. \quad (72a)$$

i.e., the excitation cross section for transitions with a quadrupole moment differs from that of transitions with dipole moment because it lacks the logarithmic factor of the order of 10 and in general has a smaller numerical factor, in accordance with Elsasser's computations of the excitation of forbidden transitions  $(1, 0) \rightarrow (n, 2)$  and  $(1, 0) \rightarrow (n, 0)$  in hydrogen.

On the contrary, in our approximation it is not possible for two electrons to be excited simultaneously by the collision process, for we have assumed that the eigenfunctions of the atom are given as the sum of the products of the electron eigenfunctions orthogonal to one another, i.e., if  $j$  enumerates the electrons, the eigenfunction of the ground state must be

$$\Psi_0 = \sum_{(\alpha)} c_{(\alpha)} \prod_j \psi_{\alpha_j}(r_j)$$

where  $\psi_{\alpha}$  must be summed over all possible permutations  $(\alpha)$ , and where the eigenfunction of the excited state must be

$$\Psi_n = \sum_{(\beta)} c_{(\beta)} \prod_j \psi_{\beta_j}(r_j)$$

Then

$$\begin{aligned} \epsilon_{n\ell}(q) &= \int \psi_n \bar{\psi}_n \sum_i e^{iqz_i} d\tau \\ &= \sum_{(m)} \sum_{(l)} c_m c_{l\ell} \int \prod_j d\tau_j \psi_{nl}(z_j) \bar{\psi}_{l\ell}(z_j) e^{iqz_j} \end{aligned}$$

and all integrals on the right side in which we do not have

$$a_j = \beta_j \text{ for all } j \neq l,$$

are zero, i.e., only one electron eigenfunction in the excited state may be changed relative to the ground state, unless all integrals are to vanish.

Furthermore, a transition to another term system of the atom cannot be excited by electron collision,<sup>\*)</sup> because perturbation by the oncoming electron is definitely symmetrical in all atomic electrons. According to Wigner [28], a transition to another term system cannot be effected by such perturbations as long as spin is not explicitly included in the computation.

### 15. Excitation of X-Ray Levels

Now we sum (71) over all possible excitations of the  $(nl)$ -electron. Taking the completeness relation of the eigenfunctions  $\psi_{nl'm}$  into consideration, we have

$$\left\{ g_{nl} \sum_{n'l'} |\psi_{nl'n'l'}(q)|^2 = \sum_n \sum_{n'l'} |\int \psi_{nlm} \bar{\psi}_{n'l'm} e^{iqz} d\tau|^2 \right. \quad (73a)$$

$$\left. - \sum_n (1 - |\int |\psi_{nlm}|^2 e^{iqz} d\tau|^2) \right.$$

$$\sum_{n'l'} |\psi_{nl'n'l'}(q)|^2 = 1 - F_{nl}^2(q) \quad (73)$$

$$F_{nl}^2(q) = |\psi_{nl'n'l'}(q)|^2 = \frac{1}{g_{nl}} \sum_n |\int |\psi_{nlm}|^2 e^{iqz} d\tau|^2 \quad (74)$$

Hence,  $F_{nl}^2(q)$  is the "atomic form factor for an  $nl$ -electron." Except for constant factors, (73) gives the intensity of the incoherent x-ray scattering or of inelastic corpuscular-ray scattering for an atom containing only one  $(nl)$ -electron. However, owing to the Pauli exclusion

<sup>\*)</sup>This is in agreement with the observation of Dymond and Watson [27].

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principle, several transitions whose matrix elements we included in (73) are forbidden: i.e., the incoherent scattering becomes relatively smaller than for an atom with one electron. From (71) we obtain directly<sup>\*)</sup>

$$\left\{ \begin{array}{l} d\Phi^{nl}(q) = \sum_{n'l'} d\Phi^{nl'}(q) = \frac{8\pi e^2}{K^2} \frac{dq}{q^2} \left(\frac{M}{m} s\right)^2 Z_{nl} \\ \cdot \left(1 - F_{nl'}^2(q) - \sum_{n''l''} \frac{\bar{Z}_{nl} Z_{n'l'} + \bar{Z}_{nl} Z_{n'l''}}{g_{n'l'} g_{n'l''}} |t_{nl, n'l'}(q)|^2\right) \end{array} \right. \quad (75)$$

or, when levels  $n'l'$  are all occupied,

$$\left\{ \begin{array}{l} d\Phi^{nl}(q) = \frac{8\pi e^2}{K^2} \frac{dq}{q^2} \left(\frac{M}{m} s\right)^2 Z_{nl} \\ \cdot \left(1 - F_{nl}^2(q) - \sum_{n'l'} |t_{nl, n'l'}(q)|^2\right). \end{array} \right. \quad (75a)$$

The total effective cross section for the excitation of an electron (especially from an inner shell) is greatly reduced in the case of small scattering angles  $\vartheta$  and collision vectors  $q$  by prohibition of transitions to occupied states, since precisely the strongest transitions are forbidden in those shells. However, in the case of large scattering angles ( $q \gg a_{nl}$ ), the matrix elements for all discrete transitions approach zero (cf. section 6); i.e., both the atomic form factor  $F_{nl}$  and the sum over the occupied states  $n'l'$  vanish, and the differential effective cross section becomes proportional to the number  $Z_{nl}$  of electrons in the  $nl$ -shell. However, collisions at a large angle contribute only slightly to the value for the integral effective cross section; on the contrary, because of the factor  $1/q^3$  in (75a), it is mainly determined by collisions with  $q \ll a_{nl}$ . Here, however, we again have (cf. (25), (38a), etc.)

$$\begin{aligned} \left| \int \psi_{nlm} \bar{\psi}_{n'l'm} e^{iqz} dz \right|^2 &\approx q^2 \left| \int x \psi_{nlm} \bar{\psi}_{n'l'm} dz \right|^2 \\ \int |\psi_{nlm}|^2 e^{iqz} dz &\approx 1 - \frac{q^2}{2} \int x^2 |\psi_{nlm}|^2 dz \end{aligned}$$

hence,

$$\lim_{q \rightarrow 0} \frac{1}{q^2} \left( 1 - F_{nl}^2(q) - \sum_{n'l'} |t_{nl, n'l'}(q)|^2 \right) = \bar{x}_{nl}^2 - \sum_{n'l'} |x_{nl, n'l'}|^2 \quad (76)$$

with

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<sup>\*)</sup>Naturally, assuming as always that practically all transitions from the  $nl$ -level are permitted, as far as energy is concerned.

$$\left\{ \begin{array}{l} \overline{x_{nl}^2} = \frac{1}{2l+1} \int x^2 \sum_n |\psi_{nlm}|^2 d\tau \\ = \frac{1}{2l+1} \int x^2 \psi_{nl}^2(r) \sum_n |P_l^n(\cos\theta)|^2 d\tau = \frac{1}{3} \int r^2 \psi_{nl}^2(r) r^2 dr \quad (76a) \\ |x_{nl,n''l''}|^2 = \frac{1}{2l+1} \sum_{n=n'}^{+1} \left| \int \psi_{nlm} \bar{\psi}_{n''l''m''} x d\tau \right|^2. \end{array} \right.$$

(The last transformation of the magnitude  $\overline{x_{nl}^2}$  presupposes that the potential field of the atom, including the eigenfunctions  $\psi_{nlm}$ , is spherically symmetric.) Integration over  $q$ , carried out in the ordinary manner (cf. sections 9, 10, and 12), yields

$$\Phi^{nl} = \frac{4\pi a^3}{K^4} \left( \frac{M}{m} z \right)^3 Z_{nl} \left( \overline{x_{nl}^2} - \sum_{n'<l'} |x_{nl,n''l''}|^2 \right) \ln \frac{2mv^2}{B_{nl}} \quad (77)$$

where  $B_{nl}$  is an energy of the order of magnitude of the ionization potential. Hence, the probability of the excitation of an ( $nl$ )-electron for outer shells is essentially proportional to the cross section of the electron shell (to the averaged square of the "distance" from the nucleus,  $r_{nl}^2$ ), but is considerably smaller for inner shells. However, the total energy transferred from the particle to the electrons of one shell is still not the same as given in sections 11 and 12. In the latter case, the outer shells benefited from the energy deficiency of the inner shells (the partial f-sums are less than 1 for inner shells and greater than 1 for outer shells). On the other hand, our excitation probability for outer shells (77) is also somewhat less (albeit only slightly) than if the inner shells were not occupied; the forbidden transitions are completely lost to the excitation probability.

If we compute the matrices  $x_{nl, n''l''}$ , introducing hydrogen eigenfunctions with a suitable effective nuclear charge  $Z'_{eff}$ , we get (cf. ref. [1, section 10]):

$$\overline{x^2} = \frac{1}{2} \frac{n^3 a^3}{Z'_{eff}} \left( \frac{3n^2 + 1}{3} - l(l+1) \right). \quad (77a)$$

That is, the approximate total excitation probability for an electron in an outer shell is roughly proportional to  $n^4$ . For inner shells in which the electrons are forbidden strong discrete transitions and essentially only the continuous transitions are still possible, we obtain

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$$\overline{x_{nl}^2} = \sum_{n''l''} |x_{nl,n'l''}|^2 = \text{about } 0.2 - 0.6 \cdot \frac{n^2 a^2}{Z_{\text{eff}}^2}, \quad (77b)$$

where the proportionality factor depends on the number and kind of the forbidden transitions, on the azimuthal quantum number  $l$ , and (only slightly) on the principal quantum number  $n$ . Since

$$\frac{R h Z_{\text{eff}}^2}{n^2}$$

is the ionization potential of the shell  $-E_{nl}$ , we can write, analogously to (53),

$$\psi^{nl} = \frac{2 n e^4 z^2}{m v^2 \cdot (-E_{nl})} \cdot Z_{nl} \cdot b_{nl} \cdot \ln \frac{2 m v^2}{E_{nl}}, \quad (78)$$

where, in very rough approximation,  $b_{nl} = 0.2$  to  $0.6$  for inner shells and is of the order of  $n^2$  for the outermost shells. Table 4 gives the excitation factors of several atoms; we used hydrogen eigenfunctions for the computation.

Table 4  
Excitation factors  $b_{nl}$

Shell	H	Be	N	Ne	A	Cu	Kr	Ag	Ne	Em
1s	1	1	0.72	0.44	0.35	0.35	0.32	0.32	0.30	0.29
2s	—	3.5	2.37	1.25	0.47	0.17	0.33	0.33	0.28	0.26
2p	—	—	1.70	1.70	1.68	0.43	0.43	0.27	0.27	0.21
3s	—	—	—	—	1.63	1.63	0.38	0.33	0.34	0.27
3p	—	—	—	—	4.55	2.05	1.98	0.56	0.55	0.33
3d	—	—	—	—	—	2.53	2.51	2.81	2.81	0.48
4s	—	—	—	—	—	—	2.12	2.12	0.61	0.36
4p	—	—	—	—	—	—	5.30	2.50	2.35	0.36
4d	—	—	—	—	—	—	—	6.40	6.32	3.16
4f	—	—	—	—	—	—	—	—	—	3.66

Equation (78) is quite critical for the intensity of the characteristic x-ray radiation emitted by the atom during bombardment with fast particles (in general, electrons), or - more exactly - for the total intensity of the lines of an x-ray series with an identical final level. The latter depend on how many electrons are removed from the inner shells of the atom; the number of these is given by (78). Hence, with high velocity bombarding electrons, the intensity of the characteristic

x-ray radiation is inversely proportional to the square of this velocity and is inversely proportional to the ionization potential. It seems that the logarithmic term, which also appears, is in even poorer agreement with Wissak's experiments (cf. [29, 30]) than is the classical Thomson formula which does not contain this term. The increase in x-ray intensity with excess of bombarding energy over the ionization potential should be even more abrupt than in Thomson's theory, while in experiment it is somewhat smoother. It must be borne in mind that our formula is not valid in Wissak's region, which lies slightly above the ionization potential. Because of the excitation factors  $b_{nf}$ , the absolute values of the excitation function appear to be lower at a small ratio of the bombarding potential to the ionization potential than in Thomson's theorem; this agrees with Wissak's experiments.

#### 16. Angular Distribution of Elastic Collisions

The number of particles deflected at an angle by elastic collisions is

$$\left\{ \begin{array}{l} d\psi_0(\vartheta) = \frac{2\pi e^4 r^3}{16 T_e^2} \sin \vartheta d\vartheta \cdot \frac{(Z - F(q))^2}{\sin^2 \frac{\vartheta}{2}} \\ q = \frac{4\pi}{\lambda} \sin \frac{\vartheta}{2} = \frac{4\pi M v}{\lambda} \sin \frac{\vartheta}{2}. \end{array} \right. \quad (23)$$

For computing the atomic form factor  $F$ , Mott [3] and Mark and Wierl [31] used the Thomas-Fermi statistical distribution of electrons in an atom and found it to be in good agreement with their experiments [32]. In this paper, we want only to compare the angular distribution of the scattered particles for scattering on heavy and light atoms, assuming the Thomas-Fermi distribution to be valid.

The number of electrons at a distance between  $r$  and  $r + dr$  from the atomic nucleus which have the nuclear charge  $Z$  is, in Fermi's notation ([33]; cf. also [34]):

$$4\pi r^2 dr \cdot \psi \bar{\psi}(r) = \frac{r dr}{e} \cdot \frac{d^3}{dr^3} (\psi(r)) = \frac{J\mu}{e} x dx \cdot \frac{d^3 \rho(x)}{dx^3},$$

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where  $v$  is the potential at point  $r$ ,  $x = r/\mu$ ,  $\varphi = x \frac{v}{\gamma}$ ,  $\gamma\mu = Ze$ ,  $\mu = \mu_0 Z^{-\frac{1}{3}}$ ,  
 $\mu_0 = \frac{\frac{2}{3}\pi^{\frac{2}{3}}}{7} \times a = 0.87a = 0.466 \times 10^{-8}$  cm, and  $\varphi(x)$  is a function computed numerically by Fermi. The atomic form factor becomes

$$\begin{aligned} F(q) &= 2\pi \int_0^\infty r^2 dr \int_0^\infty \sin \theta d\theta e^{-iqr} \cos \theta \psi(r) \\ &= 4\pi \int_0^\infty r^2 dr \psi(r) \cdot \frac{\sin qr}{qr} = Z \int_0^\infty \frac{\sin \mu_0 q x}{\mu_0 q} \frac{d^3 p}{dx^3} \cdot dx \\ &= Z \int_0^\infty \left( -\frac{d^3 p}{dx^3} \right) \cdot \cos \mu_0 q Z^{-\frac{1}{3}} x dx. \\ F(q) &= Z \tilde{\mathfrak{F}} \left( 4\pi \frac{\mu_0}{\lambda} \sin \frac{\theta}{2} Z^{-\frac{1}{3}} \right) = Z \cdot \tilde{\mathfrak{F}} \left( \frac{\sin \frac{\theta}{2}}{\lambda} Z^{-\frac{1}{3}} \right), \end{aligned} \quad (79)$$

where

$$\tilde{\mathfrak{F}}(\xi) = \tilde{\mathfrak{F}}(5.85 \xi) = \int_0^\infty \left( -\frac{d^3 p}{dx^3} \right) \cdot \cos 5.85 \xi x \cdot dx \quad (80)$$

and  $\lambda$  is in Ångströms.

Hence, according to Thomas and Fermi, the atomic form factor per electron,  $F/Z$ , becomes a universal function  $\tilde{\mathfrak{F}}$  of the argument

$$\frac{\sin \frac{\theta}{2}}{\lambda} \cdot Z^{-\frac{1}{3}}$$

and no longer depends separately on  $\frac{\sin \frac{\theta}{2}}{\lambda}$  and the atomic number  $Z$ . The function  $\tilde{\mathfrak{F}}$  is tabulated in table 5 (after Bragg [35]); it is monotonic decreasing with increasing argument. If argument  $\xi$  is small,  $\tilde{\mathfrak{F}}$  behaves as  $1 - \text{const} \times \xi^2$ , as can easily be seen from partial integration of (80):

$$\begin{cases} \tilde{\mathfrak{F}}(\xi) = -[\varphi \cdot \cos 5.85 \xi x]_0^\infty - 5.85 \xi \int_0^\infty \varphi \sin 5.85 \xi x \cdot dx \\ \lim_{\xi \rightarrow 0} \tilde{\mathfrak{F}}(\xi) = 1 - (5.85 \xi)^2 \int \varphi x dx = \text{etwa } 1 - 160 \xi^2. \end{cases} \quad (80a)$$

The same  $\frac{\sin \frac{\theta}{2}}{\lambda}$  has corresponding smaller values of argument  $\xi$  for heavy atoms than for light atoms, i.e., larger values of the atomic

form factor per electron  $\beta$ . The decrease of the atomic form factor inversely with the scattering angle is steeper in light atoms than in heavy atoms.

Table 5

$\xi = \frac{\sin \frac{\vartheta}{2}}{\lambda} Z^{-\frac{1}{3}}$	atomic form factor $\xi(\xi)$	scattering intensity according to Fermi		$\xi$	$\xi(\xi)$	scattering intensity	
		$1 - \xi$	$\frac{(2\pi r_e)^3}{1 + (2\pi r_e \xi)^2}$			Fermi	Wentzel
0	1	100	80	0,15	0,485	22,9	23,5
0,02	0,947	133	77	0,20	0,395	15,1	16,5
0,04	0,853	92	71	0,25	0,322	10,0	13,3
0,06	0,758	67	63	0,30	0,277	8,0	9,8
0,08	0,677	50,5	53	0,40	0,207	5,0	5,8
0,10	0,610	30,	44	0,50	0,156	3,4	3,8
0,12	0,550	31,5	37				

The number of particles elastically scattered in the range of angles from  $\vartheta$  to  $\vartheta + d\vartheta$  now becomes

$$d\Phi_0(\vartheta) = \frac{2\pi e^4 z^2 Z^4}{16 T_e^3 \sin^4 \frac{\vartheta}{2}} \left(1 - \xi \left(\frac{\sin \frac{\vartheta}{2}}{\lambda} Z^{-\frac{1}{3}}\right)\right)^2 \sin \vartheta d\vartheta. \quad (81)$$

As shown in refs. [13], [17, p. 231], and [36], (81) becomes the simple Rutherford formula for large angles of deflection; a "screening factor"  $(1 - \xi)^2$  is also involved when the angles are small. Since  $\xi$  is smaller and  $\xi(\xi)$  is larger for heavy atoms than for light atoms in the case of identical  $\frac{\sin \frac{\vartheta}{2}}{\lambda}$  (in contrast to Rutherford), the scattering power of heavy atoms diminishes more sharply than that of light atoms:

The decrease of the scattering intensity with the scattering angle is less steep for all atoms than according to Rutherford's formula, and even more gradual for heavy atoms than for light ones.

This theorem has been verified quite satisfactorily by the experiments of Mark and Wierl ([31]).

In making a more detailed study of the dependence of the scattering intensity on the angle, we can also combine Rutherford's factor

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$\sin^4 \frac{\vartheta}{Z}$  with  $(1 - F^2)$  to advantage:

$$\left\{ \begin{array}{l} d\Phi_0(\vartheta) = \frac{e^4 Z^2}{32 \pi^3} \left( \frac{M}{m} z \right)^2 \left( \frac{1 - F(\xi)}{\xi} \right)^2 \sin \vartheta d\vartheta \\ = 0,00356 \left( \frac{M}{m} z \right)^2 \cdot Z^2 \cdot \left( \frac{1 - F(\xi)}{\xi} \right)^2 \sin \vartheta d\vartheta, \end{array} \right. \quad (81a)$$

if the effective cross section  $d\Phi_0(\vartheta)$  is measured in  $(\text{\AA})^2$ . In the third column of table 1,  $1 - F/\xi^2$  is given as a function of

$$\xi = \frac{\sin \frac{\vartheta}{2}}{\lambda} Z^{-\frac{1}{3}}$$

Thus, this function gives the universal pattern of the decrease of scattering intensity with the scattering angle for the scattering of corpuscular radiation. For very small scattering angles, i.e., when  $\xi$  is small, (80a) holds and we have, approximately,

$$d\Phi_0(\vartheta) = 0,6 \cdot \left( \frac{M}{m} z \right)^2 Z^{\frac{2}{3}} \sin \vartheta d\vartheta (\text{\AA})^2, \quad (81b)$$

In other words, the scattering power for inelastic collisions then becomes independent of  $\vartheta$  and proportional to  $Z^{2/3}$  (rather than to  $Z^2$  when the scattering angle is large).\*)

Naturally, use of the Thomas-Fermi distribution for electrons in the atom gives better results for the scattering power than does the summing combination of all electrons in the K-shell (using Wentzel's method). Wentzel obtains

$$d\Phi_0(\vartheta) = \frac{2 \pi e^4 Z^2 \sin \vartheta d\vartheta}{16 T_e^2 \left( \sin^2 \frac{\vartheta}{2} + \left( \frac{\lambda}{2 \pi r} \right)^2 \right)^{1/2}}, \quad (82)$$

where the "atomic radius"  $r$  must be determined arbitrarily by experimentation. Then if we set  $r = r_0 Z^{-1/3}$ , ( $r_0 = \sim 1 \text{\AA}$ ), we obtain

\*) However, this requires that  $\frac{\sin \frac{\vartheta}{2}}{\lambda} Z^{-\frac{1}{3}}$  be smaller than  $0.01 Z^{\frac{1}{3}}$ , i.e., the observation must be made closer to the primary beam than the first point of interference in most metals (e.g., in Au,  $\frac{\sin \frac{\vartheta}{2}}{\lambda} = 0.037 Z^{\frac{1}{3}}$ ). Hence, no observation is possible.

$$d\Phi_0(\theta) = 0.00356 \left(\frac{M}{m} z\right)^2 \cdot Z^{\frac{2}{3}} \cdot \frac{(2\pi r_0)^2}{1 + (2\pi r_0 \xi)^2} \sin \theta d\theta. \quad (82a)$$

The function  $\frac{(2\pi r_0)^2}{1 + (2\pi r_0 \xi)^2}$ , which replaces Thomas and Fermi's  $1 - F/\xi^2$ ,

is given in table 3, column 4 for the arbitrary value  $(2\pi r_0)^2 = 80 \text{ \AA}^2$ ; with the exception of small scattering angles, it agrees to some extent with the Thomas-Fermi function. Next, the more precise expression "the effective atomic radius is proportional to  $1/\sqrt[3]{Z}$ " from Fermi's theory is introduced into Wenzel's formula, since Wentzel's formula alone tells us nothing about  $r$  or about the variation of the decrease of the scattering intensity with the angle in light and heavy atoms.\*)

### 17. Angular Distribution of Inelastic Scattering

We compute the total number of inelastically scattered particles that experience a change of momentum, of an amount between  $q$  and  $q + dq$ , due to scattering by summing the number of scatterings in the individual ( $nl$ )-shells (eq. (75)):

$$\begin{aligned} d\Phi(q) &= \sum_{nl} \sum_{n'l'} d\Phi_{n'l'}^{nl}(q) \\ &= \frac{8\pi n^2}{K^4} \frac{dq}{q} \left(\frac{M}{m} z\right)^2 \sum_{nl} \sum_{n'l'} |t_{nl, n'l'}(q)|^2 \\ &= \frac{8\pi n^2}{K^4} \frac{dq}{q} \left(\frac{M}{m} z\right)^2 \left(Z - \sum_n Z_{nl} F_{nl}^2\right. \\ &\quad \left. - \sum_{nl} \sum_{n'l'} \frac{\vec{Z}_{nl} \vec{Z}_{n'l'} + \vec{Z}_{n'l} \vec{Z}_{nl}}{g_{nl} g_{n'l'}}\right. \\ &\quad \left. \cdot \sum_n |\psi_{nlm} \bar{\psi}_{n'l'm} e^{iqz} d\tau|^2\right). \end{aligned} \quad (83)$$

\* We can say, however, that the effective atomic radius  $r$  cannot be either the radius of the K-shell or the effective radius critical for molecular distances (the former being proportional to  $Z^{-1}$ , the latter increasing with  $Z$ ), but is approximately the radius of a sphere containing, e.g., half the total charge of the atomic electrons. This radius, however, can only be obtained from a statistical theory such as that of Thomas and Fermi. Wentzel's formula, on the other hand, is justified when the validity boundaries of Rutherford's formula are to be estimated; then, for  $r$  we have to set the radius of the K-shell  $r = \frac{a}{Z}$ , because with an increasing angle  $\theta$ , the K-shell retains its scattering power longer than any other shell.

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The expression in the parentheses, which is also critical for the intensity of the incoherent x-ray scattering, has already been derived in essence by Waller and Hartree [16], who employed the completeness relation for the eigenfunction of an atom, and the expression of the eigenfunction of the ground term of the atom, as the product of two determinants containing the eigenfunctions of the individual electrons. However, Waller and Hartree did not average the matrix elements over  $m$  (which must be done because of azimuthal degeneracy); they write

$$\left| \int \psi_{nlm} \bar{\psi}_{n'l'm'} e^{iqz} d\tau \right|^2 \text{ instead of } \frac{1}{g_{nl}} \sum_{m=-l}^{+l} \left| \int \psi_{nlm} \bar{\psi}_{n'l'm'} e^{iqz} d\tau \right|^2,$$

but this is unnecessary for atoms with closed shells, which were investigated by Waller and Hartree in greater detail. For such atoms, from (83) we obtain

$$\begin{cases} d\Phi(q) = \frac{8\pi n^2}{K^3} \frac{d\eta}{q^3} \left( \frac{M}{m} z \right)^2 \left( Z - 2 \sum_{nl} (2l+1) F_{nl}^2(q) \right. \\ \left. - 2 \sum_{nl} \sum_{n'l'} \sum_m \left| \int \psi_{nlm} \bar{\psi}_{n'l'm'} e^{iqz} d\tau \right|^2 \right), \end{cases} \quad (83a)$$

where the double sum must be taken over all the occupied shells  $nl$  and  $n'l'$  and where the possibility of two spin directions accounts for the factor 2. Formulas (83) and (83a) also indicate (see section 15) that the component of forbidden transitions must be subtracted from the inelastic scattering intensity  $Z - \sum_{nl} F_{nl}^2$  computed without considering Pauli's principle.

If the scattering angle is large, the matrix elements of the forbidden transitions and the atomic form factors  $F_{nl}$  again approach zero and the scattering intensity becomes proportional to the number of electrons  $Z$ . Hence, we can state that at large angles every electron scatters classically, i.e., the energy momentum principle is satisfied for the colliding particle and the scattering electron (section 6) and the scattering cross section has the classical value for a scattering particle with the charge 1; the intensities of the scatterings of the various electrons are simply additive terms. At a large scattering

angle (vanishing atomic form factor), the ratio of inelastic (83a) to elastic scattering (81) is  $Z:Z^2$ , as in classical theory. To be sure, we have not actually compared scattering at the same angle, but rather scattering with identical momentum change of the colliding particles; converting (as in section 7) to scattering at the same angle, in analogy to (42), we obtain for large  $\delta$

$$\frac{d\Phi(\delta)}{d\Phi_e(\delta)} = \frac{Z}{Z^2} \cdot \frac{1 \cos \delta}{(1 + \cos \delta)^2} \quad (84)$$

which differs little from  $Z:Z^2$  (cf. the table for (42)). At a small scattering angle, we obtain the same result as for hydrogen: The inelastic scattering reaches a boundary value which exceeds the boundary value of the elastic scattering, e.g., in the ratio of kinetic energy of the colliding electrons to ionization potential of the atom. This agrees qualitatively with the experiments of Dymond [27] on inelastic electron scattering in He and with Arnot's experiments [37] on scattering in Hg: Inelastic scattering predominates if the angle is small, especially if the energy of the colliding electrons is large and the ionization potential is small (Hg); elastic scattering predominates at a large scattering angle. However, the inelastic scattering should be quantitatively more intensive relative to the elastic scattering than it is in the experiments, e.g., the ratio 2:4 is scarcely approached for He at large scattering angles. Of course, the electron velocities used may be too close to the ionization potential; it would be highly desirable to investigate the angular distribution of the inelastically scattered electrons at a high primary velocity. \*)

#### 18. Primary Ionization

We obtain the effective cross section for ionization in the ( $nl$ )-shell (i.e., the number of the atoms from which an ( $nl$ )-electron is removed by collision), by summing the transition probabilities (71)

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\*) Dr. Kulenkampff of the Munich Institute of Technology has informed me that such experiments are currently in progress there.

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over all states  $n'l' = k$  of the continuous spectrum and integrating over  $q$ :

$$\Phi_i^{nl} = \frac{8\pi e^3}{K^2} \left(\frac{M}{m} z\right)^3 Z_{nl} \int_0^\infty dk \int_{q_{\min}}^{q_{\max}} \frac{dq}{q} |\epsilon_{nl,k}^1(q)|^2, \quad (85)$$

$$|\epsilon_{nl,k}^1(q)|^2 = \frac{1}{g_{nl}} \sum_m \left| \int \psi_{nl,m} \bar{\psi}_{km} e^{iqx} d\tau \right|^2. \quad (85a)$$

For large  $q$

$$\int dk |\epsilon_{nl,k}^1(q)|^2 = \int |\psi_{nl,m}|^2 |e^{iqx}|^2 d\tau = 1,$$

for the discrete transitions are then no longer substantial; hence, the integrand in (85) decreases with  $1/q^3$ . Integrating in the usual manner, we obtain approximately

$$\Phi_i^{nl} N = \frac{4\pi n^3}{K^2} N \left(\frac{M}{m} z\right)^3 Z_{nl} \int dk |x_{nl,k}|^2 \ln \frac{2\pi r^2}{r_{nl}}, \quad (85b)$$

for the number of primarily-formed ( $nl$ )-ions per centimeter path (cf. section 15);  $x_{nl,k}$  is again the element of the coordinate matrix and  $C_{nl}$  an energy of the order of magnitude of the ionization potential of the ( $nl$ )-subshell, or, to conclude from the corresponding formula (54b) for hydrogen, about one power of ten smaller. Conversion analogous to that from (77) to (78) yields

$$s_{nl} = N \Phi_i^{nl} = \frac{2\pi r^3 z^3 N}{m v^3} \cdot \frac{c_{nl} Z_{nl}}{-E_{nl}} \ln \frac{2\pi r^2}{C_{nl}}, \quad (86)$$

where

$$c_{nl} = \frac{Z_{nl}^2}{n^2 m^2} \int dk |x_{nl,k}|^2 \quad (86a)$$

is a constant (ionization factor), which is computed as approximately 0.05 to 0.3 by employing hydrogen eigenfunctions:

Subshell	$1s$	$2s$	$2p$	$3s$	$3p$	$3d$	$4s$	$4p$	$4d$	$4f$	
	0,28	0,21	0,13	0,17	0,14	0,07	0,07	0,15	0,13	0,09	0,04

Subshells with a large azimuthal quantum number are more difficult to ionize than those with a small number (the extensively projecting electron of an s-shell offers, so to speak, a larger exposed surface);

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in addition, the ionization probability is approximately inversely proportional to both the ionization potential and the square of the particle velocity further multiplied by a logarithmic factor. In the case of a high primary velocity, the classical formula of Thomson [18] gives instead

$$s_{nl} = \frac{2\pi N e^4 r^2}{m v^2} \frac{Z_{nl}}{-E_{nl}} \quad (87)$$

without the logarithmic factor (cf. end of section 15).

By summation over all  $nl$ -shells of the atom, we obtain

$$s_0 = \sum_{nl} s_{nl} = \frac{2\pi e^4 r^2 N}{m v^2} \sum_{nl} \frac{c_{nl} Z_{nl}}{-E_{nl}} \ln \frac{2m v^2}{C_{nl}} \quad (88)$$

from (86) for the total number of ions formed per centimeter of path. Because of the factor  $\frac{1}{-E_{nl}}$ , the probability of ionization in inner shells is one or more orders of magnitude smaller than that in outer shells, in contrast to the stopping cross section which is smaller for inner shells by a factor  $\leq 5$  (cf. section 12). Therefore, only the ionization of the outer shells need be considered on the whole.

When (66) is divided by (88), we obtain

$$E_0 = -\frac{\frac{dT}{dx}}{s_0} = \frac{3 \sum_{nl} f_{nl} \ln \frac{mv^2}{A_{nl}}}{\sum_{nl} \frac{c_{nl}}{-E_{nl}} Z_{nl} \ln \frac{2mv^2}{C_{nl}}} \quad (89)$$

for the energy consumed per primary ion. To a certain extent, the logarithms for kinetic energies of the primary electron, which are very large in comparison with the ionization potential of the innermost shell, become equal. Rough approximation independently of  $v$  yields

$$E_0 = 2 \frac{Z J_a}{Z_a c_a}, \quad (89a)$$

where  $Z_a$ ,  $J_a$ , and  $c_a$  are the electron number, the ionization potential, and the ionization factor of the outermost shell, respectively.

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This gives \*)

$$2 \times \frac{7}{5 \times 0.13} \times 15 \approx 300 \text{ volts}$$

for N, while a more exact evaluation of (89) yields considerably less, viz., 81 volts at a primary energy of 30,000 volts. We cannot rely too heavily on this value either, since computation of the ionization factors by means of hydrogen eigenfunctions is very uncertain. It is certain, however, that the energy consumption per primary ion is a high multiple of the smallest ionization potential, as was also the case in hydrogen (a factor of 7; section 10).

The primary fault is that only a small part of the inelastic collisions leads to ionization; the larger part leads to excitation. What is more, a considerable portion of the energy supplied by the particle is consumed in excitation and ionization of inner shells, while the number of the primary ions must be furnished mainly by the ionization of the outer shells. Finally, about half of the energy is transformed into the kinetic energy of fast secondary electrons, i.e., electrons whose energy is large compared with the ionization potential.

The majority of all collision processes involving large momentum change of the colliding particle  $q \gg a_{nl}$  leads to emission of secondary electrons with momentum  $q$ , i.e., with kinetic energies that are large relative to the ionization potential. Since we can set  $Z_{nl} = f_{nl}$ , the energy lost during such collisions is approximately

$$\begin{aligned} E' &= \frac{8\pi a^3}{K^2} \left(\frac{M}{m}\right)^2 \sum_{nl} Z_{nl} \int_{a_{nl}}^{K \frac{m}{M+1}} \frac{dq}{q} \\ &= \frac{4\pi a^3}{K^2} \left(\frac{M}{m}\right)^2 \sum_{nl} Z_{nl} \ln \frac{K^2 m^2}{a_{nl}^2 M^2}, \end{aligned}$$

i.e., about half the total transferred energy  $E$ .

However, although the energy converted into kinetic energy of fast secondary electrons constitutes a large part of the total energy

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<sup>a)</sup> The ionization potential and ionization factor of the L<sub>2</sub>-subshell is assumed for all 5 L-electrons.

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lost by the colliding particle, the fast electrons, judging by their number, make up but a small fraction of all secondary electrons. By far the greatest number of secondary electrons occurs in collisions in which the particle's momentum changes only slightly ( $q \ll a_{nf}$ ) (because of the factor  $1/q^3$ ; see beginning of this section). In this case, however, the probability of formation of a secondary electron with the energy  $\frac{h^2}{8\pi^2 m} k^2$  is given by the element of the coordinate matrix corresponding to the transition from one shell of the atom to the state  $k$  of the continuous spectrum; this is of considerable magnitude only for  $k < a_{nf}$  (cf. section 6), i.e., for secondary electrons whose energy is even smaller than the ionization potential.

The velocity distribution of the secondary electrons released from hydrogen molecules is calculated roughly for a primary velocity of approximately 10,000 volts ( $\beta = 0.2$ ) and compared with Ishino's [38] data. In the computation it is assumed that the transition probabilities have the same form as in the case of the hydrogen atom and the only change required is that  $a^2$  be replaced by  $1.16 a^2$  in all formulas, because the energy  $2.32 Rh = 2 \times 1.16 Rh$  is required for removal of both the electrons of  $H_2$ . We obtain

Table 6  
Velocity distribution of the secondary electrons of hydrogen

Retarding potential in volts	Number of secondary electrons which overcome the retarding potential		
	theor.	exper.	Thomson's theorem
0	100	100	100
10	25	20,6	61
20	17	12,7	44
40	11	7,74	24
110	4,8	3,12	12,5
190	2,7	1,87	7,6
390	1,31	1,01	3,9
790	0,61	0,29	1,9
990	0,48	0,13	1,5
1100	0,42	0	1,2

Hence, the theoretically computed velocity distribution agrees quite well with experiment, in contrast to the distribution computed

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using Thomson's method; the remaining difference is caused by inclusion of the tertiary electrons (whose velocities are even somewhat smaller) in the experiments.

#### 19. Secondary Ionization

It is well known that fast secondary electrons are themselves capable of repeated ionization. Likewise, an atom with an inner shell that has been excited primarily can be ionized by an Auger jump; in addition, it emits fast secondary electrons which in turn cause ionization. Collision of one internally excited atom with another might also cause ionization. For at least an estimate of the secondary ionization, let us make two assumptions:

1. Whenever the colliding primary particle, in an elementary process, transfers an energy of more than twice the smallest ionization potential to the atom, whether in the form of inner excitation or by transfer of relatively large kinetic energy to the secondary electron, this energy can be used for the secondary excitation or ionization of another atom.
2. The secondary processes should divide into excitations and ionizations in the same manner as the primary processes; on the average, the same energy should be consumed for each ionization as must be expended by the primary particle.

The latter assumption is supported by the fact that the energy loss per formed ion (89) does not depend essentially on the velocity of the colliding particle [39]. In any case, it is more satisfactory than the earlier classical assumption by Bohr, which had to assume a complete utilization of the energy of the secondary electrons for the ionization, in contrast to conditions in the primary ionization. However, it is doubtful whether our assumption No. 2 is even roughly valid for electrons with a kinetic energy about twice the ionization potential, especially since Born's method does not apply to that case. Although our

assumptions are arbitrary, it seems that a better treatment of the very complex phenomenon of secondary ionization is not possible at present.

Hence, let  $\kappa$  be that fraction of the energy transferred from the primary particle, which according to our assumption No. 1 is available for secondary processes. It is composed of the energy converted into the kinetic energy of fast electrons (velocity greater than the smallest ionization potential) and used for the excitation of inner shells, minus twice the smallest ionization potential. However, we can omit this subtraction,<sup>\*)</sup> since it is not important for either the ionization potential of inner shells or the kinetic energy of the fast electrons, and we get approximately

$$\kappa = \frac{1}{2} + \frac{\sum' f_{nl} \ln \frac{mv^2}{A_{nl}}}{\sum f_{nl} \ln \frac{mv^2}{A_{nl}}}, \quad (90a)$$

where the primed sum is taken over the inner shells only and the unprimed sum over all shells. However, the energy consumed in the formation of one ion in the secondary processes must be of the same magnitude as in the primary processes; hence, the numerical ratio between the secondary and the primary ions must be  $\kappa:1$ . On the other hand, in the secondary processes, the fraction  $\kappa$  of the energy must be used again for excitations that can give rise to tertiary ionization, etc. Thus, the quotient of the total (primary, secondary, tertiary, etc. ionization) over the primary ionization becomes

$$\frac{s}{s_0} = 1 + \kappa + \kappa^2 + \dots = \frac{1}{1-\kappa} = \frac{2}{1 - \frac{\sum' f_{nl} \ln \frac{mv^2}{A_{nl}}}{\sum f_{nl} \ln \frac{mv^2}{A_{nl}}}}. \quad (90)$$

Hence, for atoms with no inner shells (H, He), the total ionization becomes approximately equal to twice the primary ionization; with  $N_2$  we obtain [four inner electrons,  $f_K \approx 2 \times 3/4 = 1.5$ , four middle electrons ( $L_1$ ,  $f = 2$ ), for which one cannot avoid subtracting twice the smallest ionization potential mentioned in our assumption No. 2], at

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<sup>\*)</sup>For compensation, we omit the electrons released from the outer shells through collisions with a momentum transfer  $q < a_{nl}$ , with a kinetic energy greater than the simple ionization potential.

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primary velocities of approximately 30,000 volts ( $\beta = 0.33$ ),  $\kappa \approx 0.63$ ,  $s/s_0 = 2.7$ , while Wilson's counts yield 3 to 4. In the case of heavy elements with many inner electrons, the number of the secondary processes should be slightly larger. On the other hand, it should hardly depend on the primary velocity. For all the energy used per ion formed, we obtain from (89) and (90)

$$E = \frac{-\frac{dT}{dx}}{e} = \frac{\sum f_{st} \ln \frac{mv^2}{C_{st}}}{\sum -\frac{C_{st}}{E_{st}} Z_{st} \ln \frac{mv^2}{C_{st}}}, \quad (91)$$

where the sum in the numerator (in practice also the sum in the denominator) is taken over the outer shells only. At a primary velocity of 30,000 volts, for  $N_2$

$$\bar{E} = \frac{85}{2.7} = 31.5 \text{ volts}$$

i.e., almost exactly the same as Eisl's experimental value (32 volts). Furthermore,  $\bar{E}$ , as in experiment, is almost completely independent of the primary velocity: at 10,000 volts,  $\bar{E} = 30$  volts. To be sure, the numerical agreement with experiment may be partly coincidental, since the more thoroughly substantiated stopping cross section (section 13) agrees less well, yet we can be well satisfied with the correlation.

## 20. Summary of the Results

1. The number of the inelastic collisions of a fast, charged particle with an atom is proportional to the intensity of the Compton effect for x-rays, which have the same wavelength and undergo the same deflection  $\delta$  as the particle divided by the Rutherford factor  $\sin^4 \frac{\delta}{2}$  (section 5).

2. In most inelastic collisions, the colliding particle is only slightly deflected: the sine of the mean deflection angle for inelastically scattered electrons is approximately equal to the root of the ionization potential divided by the kinetic energy of the electron (section 6)

$$\bar{q} \approx K \sin \bar{\varphi} \approx a_{st}, \sin \bar{\varphi} \approx \frac{a_{st}}{K} = \sqrt{\frac{-E_{st}}{\frac{1}{2} m v^2}}$$

3. In inelastic collisions with large deflection, the momentum principle for colliding particles and secondary electrons is nearly satisfied, in which case the nucleus of the atom is not involved (section 6).

4. In the case of large deflection angles, the number of the inelastic collisions is related to the number of the elastic collisions as  $Z:Z^2$ ; if the deflection angles are small, the number of the inelastic collisions is larger than that of the elastic collisions by approximately the factor "kinetic energy of the particle divided by ionization potential of the atom" (sections 17 and 7).

5. The dependence of the number of the elastic collisions on the scattering angle can be represented by a universal function of  $\frac{\sin \frac{\theta}{2}}{\lambda \sqrt{Z}}$ , using the Thomas-Fermi distribution for the electrons in the atom. The decrease of the collision count with increasing angle is more gradual for heavy atoms than for light atoms, in agreement with the experiments of Mark and Wierl; with a large scattering angle, the collision count is proportional to  $Z^2$ , and with a small angle, proportional to  $Z^{2/3}$  (section 16).

6. The probability for the excitation of a certain transition of the atom due to collision of fast electrons is almost exactly proportional to the optical transition probability for this transition and inversely proportional to the kinetic energy of the electrons. Therefore, nearly all collisions cause excitation of the resonance line (sections 14, 5, and 9).

7. The probability of the excitation of an x-ray level (ionization of an atom in an inner shell) through collision of fast electrons is, in first approximation, inversely proportional to the ionization potential of the excited level and the kinetic energy of the electrons. Besides, a logarithmic term appears, which is not found in the classical theory (section 15).

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8. The stopping cross section of an atom for  $\alpha$ -particles and electrons is inversely proportional to the square of the velocity of the particle and proportional to a logarithmic term whose argument does not exactly agree with the one known from Bohr's theory (sections 12, 13, and 10).

9. The stopping cross section of an atom is composed additively of the stopping cross sections of the individual electron shells. The latter are proportional to the sum of the oscillator strengths of all transitions that can be made by the electrons of the shell rather than to the number of the electrons in each shell. The stopping cross section of an electron in an outer shell is greater than in an inner shell by a factor of 3 to 5 (section 12).

10. The stopping cross section for very fast electrons should be approximately proportional to  $Z$ ; for slower electrons and for  $\alpha$ -particles, it increases more slowly with  $Z$ . An explicit law cannot be given for this increase. The theoretical values for the stopping cross section seem to increase somewhat more rapidly with  $Z$  than do the experimental values. Theory and experiment are in agreement for the elements up to argon (section 13).

11. The stopping cross section of heavy atoms decreases more gradually with increasing velocity than that of light atoms; therefore, in a substance of high atomic weight, the range of a particle is proportional to a low power of the velocity, in agreement with observation. For very large velocities, the range is always proportional to  $v^4$ . The proportionality factor (the constant of the Thomson-Whiddington law) is slightly too high (section 13).

12. The number of primarily formed ions per centimeter of path formed by a fast particle is inversely proportional to the square of the velocity of the particle, inversely proportional to the ionization potential of the atoms, and proportional to a logarithmic term which is not found in the classical theory. In the argument of the

logarithm, the square of the particle velocity is divided by the smallest ionization potential of the atom (sections 18 and 19).

13. The ratio of the number of all the ions formed to the primary ions is, starting from a certain lower limit, almost independent of the velocity of the ionizing particle and increases from slightly more than 2:1 in hydrogen to approximately 3:1 in air and even more in heavy elements. In agreement with this, the experiments of Wilson give a ratio 3 to 4:1 for air (section 19).

14. The energy consumption for every primary ion in hydrogen, for very high velocities of the colliding particle, is greater by a factor of approximately 7 than the smallest ionization potential, and for heavier atoms the factor is even larger. For every ion formed (either primary or secondary), the energy consumption must be nearly independent of the velocity; for air, it is approximately 32 volts, in agreement with observation (sections 18, 19, and 10).

15. By far most of the secondary electrons have a kinetic energy of the order of magnitude of the simple ionization potential or even less. However, about half of the energy imparted by the colliding particle is converted into kinetic energy of fast secondary electrons (section 19).

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**On the Theory of Metals, I. Eigenvalues and Eigenfunctions  
of a Linear Chain of Atoms**  
*Zeits. Physik* 71, 205–226 (1931)

The atoms are supposed to have spin 1/2. Only neighbors interact, and the interaction is supposed to be attractive if their spins are parallel, repulsive if opposite. The assumptions are thus similar to the Ising model, but the spins are treated properly by quantum mechanics. An assumption is made about the eigenfunction; this has been much used in quantum statistics and is known as “Bethe’s Ansatz”.

# ON THE THEORY OF METALS, I. Eigenvalues and Eigenfunctions of a Linear Chain of Atoms

by H. Bethe in Rome

(Dated 13 June, 1931; received 17 June, 1931)

A method is given whereby the zero-order eigenfunctions and first-order eigenvalues (in the sense of the London-Heitler approximation scheme) are calculated for a one-dimensional "metal" consisting of a linear chain of a very large number of atoms, each of which has a single  $s$ -electron with spin, outside closed shells. In addition to the spin waves of Bloch, bound states are found, in which parallel spins are predominantly on nearest neighbor atoms; these features may be important for the theory of ferromagnetism.

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*Translated in 1992 from Zeitschrift für Physik, vol. 71, pp. 205-226 (1931)  
by Vince Frederick : a small number of misprints in the original paper  
have been corrected, the terminology has been brought somewhat  
up-to-date and footnotes renumbered, by the Editor.*

§1. Until now, the theory of metals has for some time been limited to the investigation of the motion of individual conduction electrons in the potential field of the metal atoms (Sommerfeld, Bloch.) The interaction of electrons with one another has been ignored, at least insofar as the electronic-interaction potentials are concerned. Although this procedure has been very fruitful in problems of metallic conductivity (with the exception of superconductivity,) it did not allow for a deeper penetration into the problem of ferromagnetism<sup>1</sup> and for example, it rendered the calculation of the cohesive forces in metals a completely hopeless undertaking: exchange forces among the conduction electrons dominate first order perturbation theory and have the same order of magnitude as the zero-point energy of the electron gas (the energy in zeroth-order perturbation theory.) Accordingly, one estimates that the second-order approximation will again be of the same order of magnitude, and so on. Under such circumstances, one should be skeptical of an approximation in which the motional energy of the electrons (kinetic zero-point energy) is considered to be overwhelmingly more important than their interaction energy (exchange energy.)

It is for such reasons that Slater<sup>2</sup> and Bloch<sup>3</sup> have recently tried to approximate the problem from another angle, that is assuming the atomic structures to be given and their interactions to be the perturbation, in accordance with the London-Heitler approximation for molecules. Slater was

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<sup>1</sup> F. Bloch, Zeit. f. Phys. 57, 545 (1929) shows that under certain assumptions "free" electrons also can exhibit ferromagnetism

<sup>2</sup> J.C. Slater, Phys. Rev. 35, 509 (1930)

<sup>3</sup> F. Bloch, Zeit. f. Phys. 61, 206 (1930)

mainly interested in the cohesive energy of non-ferromagnetic materials, in which the London-Heitler exchange integral is generally negative<sup>4</sup> [editor's note: here,  $J < 0$  implies *antiferromagnetic* couplings], and gave an interesting method for the approximate calculation of the ground state energy of such metals when the total spin vanishes. In the case of ferromagnetism, Bloch calculated approximately the leading terms in the opposite case  $J > 0$  [editor's note:  $J > 0$  implies *ferromagnetic* couplings] in a systematic fashion, but obtained too many eigenvalues by his method. It is the aim of the present work first, to give a procedure for the case of a linear chain of atoms, which allows the calculation of every eigenvalue of this one-dimensional crystal to arbitrary accuracy within the context of the first approximation of the London-Heitler method, such that the problem will be at exactly the same stage as the Hydrogen molecule  $H_2$  in the London and Heitler work. And in addition, to obtain other types of solutions differing from the (somewhat modified) Bloch<sup>3</sup> solutions, ensuring that the total number of eigenvalues turns out exactly correct.

§2. Our problem can be stated as follows: given a linear chain composed of a large number ( $N$ ) of like atoms where each atom has a single valence electron in an  $s$ -orbit outside closed shells occupying a known atomic eigenfunction, what are the zeroth-order eigenfunctions and first-order eigenvalues of the entire system when the interactions among the individual atoms is taken into account?

As long as one neglects the interaction energies, there are 2 states of equal energy for each atom—the spin of the valence electron can point either

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<sup>4</sup> W. Heisenberg, Zeit. f. Phys. **49**, 619 (1928)

right or left. The energy eigenvalue of the chain is therefore  $2^N$ -fold degenerate in zeroth approximation. Each of these states of the chain can be specified by enumerating the atoms which carry a right-handed spin; assume this to be the case for the atoms  $m_1, m_2, \dots, m_r$ . The corresponding totally antisymmetric eigenfunction of the chain is  $\phi(m_1, m_2, \dots, m_r)$ . The correct zeroth-order eigenfunctions therefore assume the form

$$\Psi = \sum_{m_1, m_2, \dots} a(m_1, m_2, \dots, m_r) \phi(m_1, m_2, \dots, m_r)$$

where each of the integers  $m_1, m_2, \dots, m_r$  runs from 1 to  $N$ . We specialize to  $m_1 < m_2 < \dots < m_r$ .

One calculates matrix elements of the interaction energy using these states, each specified by its spin distribution  $m_1, m_2, \dots, m_r$ , obtaining:<sup>3</sup>

*Diagonal Elements:* if in the spin distribution  $m_1, m_2, \dots, m_r$  there are  $N'$  nearest neighbor pairs of parallel spins, then  $W_{m_1, m_2, \dots} = E_0 - N'J$ .  $E_0$  is the electrostatic interaction energy of the atoms and  $J$  is the London-Heitler exchange integral between two neighboring atoms. Exchange integrals for non-nearest-neighbor atoms are neglected, as they fall off exponentially with distance.

*Nondiagonal Elements* occur between any two states which differ merely by a single permutation of a pair of adjacent antiparallel spins as, for example, between  $m_1, \dots, m_j, \dots, m_r$  (where we suppose  $m_j+1$  to be a left-handed spin and therefore missing from the enumeration) and  $m_1, \dots, m_{j+1}, \dots, m_r$ . (with  $m_j$  missing). All such off-diagonal matrix elements have a value  $-J$ .

With the aid of the interaction matrix elements, one obtains the following equations among the coefficients  $a(m_1 \dots m_r)$  of the eigenstate  $\Psi$

which we are seeking:

$$2\epsilon a(m_1 \dots m_r) + \sum a(m'_1 \dots m'_r) - a(m_1 \dots m_r) = 0 \quad (1)$$

Here,

$$2\epsilon J = \epsilon - E_0 + NJ \quad (2)$$

and  $\epsilon$  is the total first-order perturbation energy. The summation is over all sets  $m'_1 \dots m'_r$  which differ from  $m_1 \dots m_r$  by a single permutation of nearest-neighbor antiparallel spins.<sup>5</sup>

In addition to Eqs.(1), the  $a$ 's must satisfy periodic boundary conditions:

$$a(m_1 \dots m_j \dots m_r) = a(m_1 \dots m_j + N \dots m_r) \quad . \quad (3)$$

§3. For  $r=1$  the solution of (1) is:

$$a(m) = e^{ikm}$$

$$\epsilon = 1 - \cos k$$

$$k = 2\pi\lambda/N, \quad \lambda = \text{integer} \quad .$$

For  $r=2$ , two cases are to be distinguished: either the two right-handed spins are separated, in which case

$$-2\epsilon a(m_1 m_2) =$$

$$a(m_1+1, m_2) + a(m_1-1, m_2) + a(m_1, m_2+1) + a(m_1, m_2-1) - 4a(m_1 m_2) \quad (4a)$$

with  $m_2 \neq m_1+1$ , or else they are adjacent, and:

$$-2\epsilon a(m_1 m_1+1) = a(m_1-1, m_1+1) + a(m_1, m_1+2) - 2a(m_1, m_1+1) \quad . \quad (4b)$$

The first set of equations are rigorously solved by an ansatz,

$$a(m_1 m_2) = c_1 e^{i(f_1 m_1 + f_2 m_2)} + c_2 e^{i(f_2 m_1 + f_1 m_2)}, \text{ and } \epsilon = 1 - \cos f_1 + 1 - \cos f_2 \quad (5)$$

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<sup>5</sup> Eq.(1) is more extensively derived by Bloch in Eq.(5) of ref. 3, where he labels atoms  $f_i$  instead of  $m_i$ , and instead of  $2\epsilon J$ , simply writes  $\epsilon$ .

in which  $c_1, c_2, f_1, f_2$  are as yet undetermined by all this.

The second set can be satisfied by selecting  $c_1$  and  $c_2$  so as to satisfy

$$0 = a(m_1, m_1) + a(m_1+1, m_1+1) - 2a(m_1, m_1+1) . \quad (6)$$

Here,  $a(m_1, m_1)$  has no physical meaning but, rather, is to be defined by (5).

Obviously, by adding (6) to (4b) we bring it to the form (4a), and we have already satisfied equations of this type. Inserting (6) into (5) yields:

$$e^{i(f_1+f_2)m_1} [c_1(1+e^{i(f_1+f_2)} - 2e^{if_2}) + c_2(1+e^{i(f_1+f_2)} - 2e^{if_1})] = 0, \quad (7)$$

$$\frac{c_1}{c_2} = -\frac{\cos(1/2)(f_1+f_2) - e^{i(1/2)(f_1-f_2)}}{\cos(1/2)(f_1+f_2) - e^{-i(1/2)(f_1-f_2)}} = \frac{\sin(1/2)(f_1-f_2) + iC_{12}}{\sin(1/2)(f_1-f_2) - iC_{12}}$$

$$\text{with } C_{12} = \cos(1/2)(f_1+f_2) - \cos(1/2)(f_1-f_2) [= -2\sin f_1/2 \sin f_2/2 .]$$

[Editor's note:  $|c_1/c_2| = 1$ , therefore we just seek a phase factor.]

Set  $c_1 = e^{i\phi/2}$ ,  $c_2 = e^{-i\phi/2}$ , so that

$$\cot \phi/2 = \frac{\sin(1/2)(f_1-f_2)}{C_{12}},$$

$$2 \cot \phi/2 = \cot f_1/2 - \cot f_2/2 . \quad (8)$$

Thus, one obtains

$$a(m_1, m_2) = e^{i(f_1m_1 + f_2m_2 + \phi/2)} + e^{i(f_2m_1 + f_1m_2 - \phi/2)} . \quad (9)$$

Additionally, it is assumed that  $m_1$  and  $m_2$  lie in the fundamental period of the chain, i.e.  $1 \leq m_1 < m_2 \leq N$ . Periodic boundary conditions require:

$$a(m_1, m_2) = a(m_2, m_1 + N) \quad (10)$$

[The notation  $a(m_2, m_1 + N)$  is explained by our convention of listing the  $m_i$  in the order of increasing magnitude, see above.] Insert (9) into (10):

$$\begin{aligned} & e^{i(f_1 m_1 + f_2 m_2 + \phi/2)} + e^{i(f_2 m_1 + f_1 m_2 - \phi/2)} \\ & = e^{i(f_1 m_2 + f_2(m_1 + N) + \phi/2)} + e^{i(f_2 m_2 + f_1(m_1 + N) - \phi/2)} \end{aligned}$$

As these must hold for all  $m_1$  and  $m_2$ , the first term on the left must be equal to the second term on the right, as they have the same dependence on  $m_1$  and  $m_2$ , and conversely, so that

$$Nf_1 - \phi = 2\pi\lambda_1, \quad Nf_2 + \phi = 2\pi\lambda_2, \quad \text{and} \quad \lambda_1, \lambda_2 = 0, 1, 2, \dots, N-1. \quad (11)$$

Although, individually, the  $f_1$  and  $f_2$  do not have the usual form  $2\pi\lambda/N$ , their sum,

$$k = f_1 + f_2 = 2\pi(\lambda_1 + \lambda_2)/N. \quad (12)$$

is a true constant of the motion of the problem; the coefficient  $a(m_1, m_2)$  is multiplied by  $e^{ik}$  if both the right-handed spins are displaced by one atomic position to the right, a translation which obviously does not affect any physical properties [by translation invariance.]

We now discuss the behavior of the phase  $\phi$  as a function of  $f_1$  and  $f_2$ , for which we specify that

$$-\pi \leq \phi \leq +\pi. \quad (13)$$

If one interchanges  $f_1$  and  $f_2$ , then clearly  $\phi$  changes sign and the coefficients remain unchanged, according to (9). If  $f_2$  is held fixed and  $f_1$  is allowed to increase from zero, then  $\cot \phi/2$  falls from  $+\infty$  to smaller positive values, finally reaching zero for  $f_1=f_2$ ; thus,  $\phi$  ranges from 0 to  $\pi$ .

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If  $f_1$  becomes slightly greater than  $f_2$ ,  $\phi$  jumps from  $+\pi$  to  $-\pi$ , gradually increasing back to zero as  $f_1$  increases to  $2\pi$ . If  $f_1=f_2$ , then either

$$\phi=+\pi, \quad \lambda_1 = \lambda_2 - 1 = Nf_1/2\pi - 1/2,$$

or

$$\phi = -\pi, \quad \lambda_1 = \lambda_2 + 1 = Nf_1/2\pi + 1/2.$$

In either instance, according to (9) for all  $m_1, m_2$ ,  $a(m_1 m_2)$  becomes

$$a(m_1 m_2) = e^{if_1(m_1+m_2)} (e^{i\pi/2} + e^{-i\pi/2}) = 0.$$

This means that  $f_1 = f_2$  [Editor's note:  $\lambda_1 = \lambda_2 \pm 1$ ] does not lead to a meaningful solution of the problem, and if  $\lambda_2$  is specified,  $\lambda_1$  can take on only the values

$$\lambda_1 = 0, 1, 2, \dots, \lambda_2 - 2, \lambda_2 + 2, \dots, N-1.$$

As  $f_1, f_2$  and  $f_2, f_1$  yield the same eigenfunction, we can specify  $f_1 < f_2$  without loss of generality. Thus for fixed  $\lambda_2$ , there are  $\lambda_2 - 1$  solutions  $\lambda_1 = 0, 1, \dots, \lambda_2 - 2$  and  $\lambda_2$  goes from 2 to  $N-1$ , so that the total number becomes:

$$\sum_{\lambda_2=2}^{N-1} (\lambda_2 - 1) = \binom{N-1}{2} = (N-1)!/2!(N-3)!$$

a binomial coefficient. Clearly, there must be as many solutions as there are distinct configurations for  $m_1$  and  $m_2$ , namely  $N!/2!(N-2)!$ . So in fact the foregoing exact analysis yields an *insufficient number* of solutions, whereas Bloch<sup>3</sup> believed that the method yields too many, namely  $(N+1)!/2!(N-1)!$ .

§4. There must exist  $N-1$  additional solutions. These are obtained by allowing the wave numbers  $f_1$  and  $f_2$  to take on complex-conjugate values. In fact we shall find that for each, arbitrary, value of  $k=f_1+f_2$  there is found precisely one pair of complex conjugate solutions to Eqs.(8) and (11) [Editor's note: the *bound-state*.] Let

$$f_1 = u + iv, \quad f_2 = u - iv, \quad (14)$$

then

$$\cot f_1/2 = \frac{\cos u/2 \cosh v/2 - i \sin u/2 \sinh v/2}{\sin u/2 \cosh v/2 + i \cos u/2 \sinh v/2} = \frac{\sin u - i \sinh v}{\cosh v - \cos u} \quad (15)$$

By (11),

$$N(f_1-f_2) = 2Niv = 2\pi(\lambda_1-\lambda_2) + 2\phi$$

$$\text{with } \phi = \psi + i\chi, \quad \psi = \pi(\lambda_2 - \lambda_1), \quad \text{and } \chi = Nv. \quad (16)$$

If  $v$  is finite, then  $\chi$  must be very large, such that

$$\begin{aligned} \cot \phi/2 &\approx \frac{\sin \psi - 1/2 e^{\chi}}{1/2 e^{\chi} - \cos \psi} = -i + 2 e^{-\chi} (\sin \psi - i \cos \psi) \\ &= -i(1 + 2 e^{-\chi+i\psi}) . \end{aligned} \quad (17)$$

In *first* approximation, the following holds:

$$\begin{aligned} 2 \cot \phi/2 &= \cot f_1/2 - \cot f_2/2 = -2i \\ &= \frac{\sin u - i \sinh v}{\cosh v - \cos u} - \frac{\sin u + i \sinh v}{\cosh v - \cos u} \\ \sinh v &= \cosh v - \cos u, \quad \text{i.e.} \quad e^{-v} = \cos u \end{aligned} \quad (18)$$

and

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$$\begin{aligned}
 \epsilon &= 2 - \cos(u+iv) - \cos(u-iv) \\
 &= 2 - 2 \cos u \cosh v = 2 - \cos u(\cos v + 1/\cos v), \\
 \epsilon &= \sin^2 u = 1/2(1 - \cos 2u). \tag{19}
 \end{aligned}$$

Clearly,  $\cos u$  has to be  $\geq 0$ , that is  $-\pi/2 \leq u \leq \pi/2$ . If then  $k = 2u + 2n\pi$  (n an integer) is between 0 and  $\pi$ , then  $u = k/2$ ,

if between  $\pi$  and  $2\pi$ , then  $u = k/2 + \pi$ .

In a second approximation we set  $v = v_0 + \epsilon$ , (20)

where  $v_0$  is value obtained in the first approximation. Then,

$$\begin{aligned}
 2 \cot \psi/2 &= -2i - 4i e^{-X+i\psi} = -2i (\sinh v) / [\cosh v - \cos u] \\
 &= -2i \frac{\sinh v_0}{\cosh v_0 - \cos u} \left[ 1 + \epsilon \left( \frac{\cosh v_0}{\sinh v_0} - \frac{\sinh v_0}{\cosh v_0 - \cos u} \right) \right] \\
 &= -2i \cdot 1 \cdot \left[ 1 + \epsilon \cdot \left( \frac{1 + \cos^2 u}{1 - \cos^2 u} - 1 \right) \right] = -2i(1 + 2\epsilon \cot^2 u),
 \end{aligned}$$

$$\epsilon = (\tan^2 u) e^{-X+i\psi}.$$

As  $\epsilon$  is in general very small,  $Nv_0$  can be written for  $X$ .  $\psi$  is now adjusted according to the prescribed value of  $k$ : if

$Nk/2\pi = \lambda_1 + \lambda_2 = \lambda$  is even and smaller than  $N/2$ , we can set

$$\lambda_1 = \lambda_2 = \lambda/2, \quad \psi = 0.$$

Likewise, for  $\lambda \geq N/2$ ,  $N + \lambda$  even:

$$\lambda_1 = \lambda_2 = (N+\lambda)/2, \quad \psi = 0.$$

If either  $\lambda$  or  $N+\lambda$  is odd, then we must write:  $\lambda_2 = \lambda_1 + 1, \psi = \pi$ .

$$\text{From this, } \epsilon = \pm \tan^2 u e^{-Nv_0} \quad (21)$$

For even  $\lambda$  (or  $N+\lambda$ ),  $v > v_0$ . If in the next approximation  $v_0$  is replaced by  $v$  then the resulting  $\epsilon$  is smaller than that of the second approximation. The procedure for the determination of  $v$  always converges, indeed very rapidly. On the other hand, if a negative sign be chosen (odd  $\lambda$  or  $N+\lambda$ ) then  $v < v_0$  and absolute value of  $\epsilon$  increases in higher approximations. This makes no difference so long as  $v_0$  is finite, as then the correction to  $\epsilon$  is infinitesimal. But if  $u$  is small and therefore  $\cos u \approx 1$ , then  $v_0$  is also small, and to sufficient accuracy

$$v_0 = -\log \cos u = 1 - \cos u = u^2/2.$$

If  $u$  is small of order  $1/\sqrt{N}$ , then  $Nv_0$  is finite and

$$\epsilon = -u^2 e^{-Nv_0}$$

is larger than  $v_0$  in absolute value so long as  $Nv_0 < \log 2 \approx 0.7$ ,  $u^2 < 1.4/N$ . For  $u < \sqrt{1.4/N}$  and odd  $\lambda$ , then  $v_1 = v_0 + \epsilon$  will be negative, the process diverges, and no solution with two complex conjugate wave numbers can be found.<sup>6</sup>

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In its place, there occurs an additional solution with two real wave numbers. We again consider  $k$  as given and  $f_2 = k - f_1$ . Earlier in the discussions of real solutions it was tacitly assumed that with increasing  $f_1$ ,  $F = Nf_1 - \phi$  increased monotonically. This might seem obvious, insofar as  $f_1$  is multiplied by a very large factor  $N$  and  $\phi$  is  $O(1)$ . Nevertheless, this assumption is invalid at small  $k$ . Looking at (8) in some greater detail, we

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<sup>6</sup> In fact, this occurs already for  $u < 2/\sqrt{N}$ , despite that in the second approximation  $v$  is positive, because higher approximations push it down to negative values.

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obtain  $dF/df_1 = N - 2 A/D$ , where  $A = (4\sin^2 f_1/2)^{-1} + (4\sin^2(k-f_1)/2)^{-1}$  and  $D = 1 + [(1/2)\cot f_1/2 - (1/2)\cot(k-f_1)/2]^2$ ; setting  $f_1 = f_2 = k/2$ , then clearly  $dF/df_1 = N - 1/\sin^2 f_1/2$  is positive only so long as  $\sin f_1/2 > 1/\sqrt{N}$ . For  $k < 4 \sin^{-1}(1/\sqrt{N}) \approx 4/\sqrt{N}$  the increase of  $F = Nf_1 - \Phi$  as function of  $f_1$  is broken off by a decrease in the vicinity of  $f_1=k/2$ . If  $Nk/2\pi = \lambda$  is odd, then

$$Nk/2 - \pi = 2\pi\lambda_1 = 2\pi(\lambda-1)/2$$

where  $\lambda_1$  is an integer, and for  $\lambda_1 = (\lambda-1)/2$ ,  $\lambda_2 = (\lambda+1)/2$ , there are two<sup>7</sup> solutions of the system of equations (8) and (11): besides  $f_1=f_2$ ,  $\Phi=\pi$ , there exists a solution  $f_1 < f_2$ ,  $\Phi \neq \pi$ , for which the coefficients (9) remain finite in contrast to the first solution.

To actually find this solution, we put  $f_1 = f - 2\epsilon/N$  and throughout and use  $\sin f = f$ ,  $\cos f = 1$ ,  $\cot f = 1/f$ , valid for small  $f$ . Then

$$2 \cot \Phi/2 = 2(f-2\epsilon/N)^{-1} - 2(f+2\epsilon/N)^{-1} = 8\epsilon/Nf^2 \quad (8a)$$

$$2\Phi = 2\pi(\lambda_2 - \lambda_1) - N(f_2 - f_1) = 2\pi - 4\epsilon \quad (11a)$$

$$\cot \Phi/2 = \tan \epsilon,$$

$$(\tan \epsilon)/\epsilon = 4/Nf^2 \quad (22)$$

From this,  $\epsilon$  is determined,  $\epsilon$  is  $< \pi/2$ , therefore  $\Phi > 0$  and  $Nf_1 > 2\pi\lambda_1$ .

With this, we have determined an additional solution, with real or complex wave number, at each value of  $\lambda$ . The largest allowed value of  $\lambda$  is obviously  $N-2$  with  $\lambda_1 = \lambda_2 = N-1$ ; for  $\lambda = N-1$  on the other hand,  $\lambda_2$  would equal  $N$ , outside the permissible interval.<sup>8</sup> Thus, we find  $N-1$  solutions  $\lambda = 0, 1, 2, \dots, N-2$ , precisely the required number.

<sup>7</sup> One can show that  $F$  can assume no other integer value more than once (for odd  $\lambda$ ) and none at all for even  $\lambda$

According to Eqs.(9),(12),(16a), the coefficients  $a(m_1 m_2)$  of our complex solutions are:

$$a(m_1 m_2) = e^{iu(m_1+m_2)} (e^{v(m_1-m_2+N/2)} \pm e^{v(m_2-m_1-N/2)}),$$

$$a(m_1 m_2) = e^{iu(m_1+m_2)} \cdot \{\text{cosh or sinh}\} v(N/2 - (m_2 - m_1)) \quad (23)$$

with  $\text{cosh}$  or  $\text{sinh}$  applying according to whether  $\lambda$  (or  $N+\lambda$  for  $\lambda > N/2$ ) is even or odd. For our solutions it is most probable that both right-handed spins lie as close together as possible, as the probability  $|a(m_1 m_2)|^2$  falls off exponentially with distance  $m_2 - m_1$ . The extreme case occurs for the solution with  $\lambda=N/2$ ,  $u = \pi/2$  and  $v=\infty$ . Here, after appropriate normalization,

$$a(m_1 m_2) = 0 \text{ for } m_2 \neq m_1 + 1, \text{ and } (-1)^{m_1}, \text{ for } m_2 = m_1 + 1,$$

and both spins are always precisely adjacent.

Every eigenvalue  $\epsilon$  for a solution with two complex conjugate wave numbers is *smaller* than any eigenvalue with the same total wave number  $k$  and real wave numbers, as we shall now show. According to (2) then, the corresponding energy  $e$  in the first approximation is *lower* than all the solutions with real wave numbers if the exchange integral  $J$  is positive (for ferromagnetism) or higher, if  $J$  is negative (the usual case.)

For the complex solution we have, specifically,

$$\epsilon_k = \sin^2 u, \quad (19)$$

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<sup>8</sup> The solution  $\lambda_1 = N-1$ ,  $\lambda_2 = N$  has, in fact, already been counted once, in the form  $\lambda_2=0$ ,  $\lambda_1=N-1$

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whereas for the real,

$$\epsilon_r = 1 - \cos f_1 + 1 - \cos (k-f_1) \quad (5)$$

(5) reaches its minimum for

$$f_1 = k/2 \text{ for } 0 \leq k \leq \pi \text{ and } f_1 = k/2 + \pi, \text{ for } \pi \leq k \leq 2\pi,$$

that is, generally for  $f_1=f_2=u$ . The minimum is

$$\epsilon_{\min} = 2(1-\cos u),$$

so that

$$\epsilon_k / \epsilon_{\min} = (1/2)(1+\cos u) \leq 1 \quad , \quad (24)$$

where the equal sign applies only at  $u=0$ .<sup>9</sup> QED.

§5. We turn now to the general case of  $r$  right-handed spins.

Eqs.(1) again fall into two types:

If none of the  $r$  designated spins  $m_1, \dots, m_r$  are adjacent, then

$$-2\epsilon a(m_1 \dots m_j \dots m_r) = \sum_{i=1}^r [a(m_1 \dots m_j + i \dots m_r) + a(m_1 \dots m_j - 1 \dots m_r) - 2a(m_1 \dots m_j \dots m_r)]. \quad (24a)$$

If instead, two are adjacent, say  $m_{k+1} = m_k + 1$ , then,

$$\begin{aligned} -2\epsilon a(m_1 \dots m_j \dots m_k m_k + 1 \dots m_r) &= a(m_1 \dots m_j \dots m_k - 1 m_k + 1 \dots m_r) \\ &\quad + a(m_1 \dots m_j \dots m_k m_k + 2 \dots m_r) - 2a(m_1 \dots m_j \dots m_k m_k + 1 \dots m_r) \\ &\quad + \sum_{i \neq k, k+1} [a(m_1 \dots m_j + i \dots m_r) \\ &\quad + a(m_1 \dots m_j - 1 \dots m_r) - 2a(m_1 \dots m_j \dots m_r)] \end{aligned} \quad (24b)$$

and analogously for any larger number of adjacent right-handed spins.

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<sup>9</sup> As  $f_1$  is never exactly equal to  $f_2$  (cf. §3), in fact the inequality always applies

We next suppose [Editor's note: "Bethe's ansatz"]:

$$a(m_1 \dots m_r) = \sum_{P=1}^{r!} \exp i \left[ \sum_{k=1}^r f_{Pk} m_k + (1/2) \sum \phi_{Pk} P_n \right] \quad (25)$$

$$\epsilon = \sum_{k=1}^r (1 - \cos f_k) \quad (26)$$

$P$  is any permutation of the  $r$  numbers 1, 2, ...,  $r$ , and  $P_k$  is the number which replaces  $k$  under this permutation. The ansatz satisfies the first set of equations (24a) by inspection. The remaining equations are satisfied by requiring that

$$2a(m_1 \dots m_k m_k + 1 \dots m_r) = a(m_1 \dots m_k m_k \dots m_r) + a(m_1 \dots m_k + 1 m_k + 1 \dots m_r) \quad (27)$$

in which the [Editor's note: *unphysical*] amplitudes on the right are to be defined according to (25). Eq.(27) must hold for any arbitrary set of  $m_1, \dots, m_r$  of which an arbitrary number can be nearest-neighbors, provided only  $m_1 < m_2 < \dots < m_r$ . All the relations (24b) are simultaneously satisfied by this device, including cases in which the  $m_1, \dots, m_r$  involve more than one pair of adjacent parallel spins; all equations are reduced to the type (24a), which have already been solved. Eq.(27) itself is satisfied by requiring the phases  $\phi$  to satisfy the relations,

$$2 \cot \phi_{kn}/2 = \cot f_k/2 - \cot f_n/2 : -\pi \leq \phi_{kn} \leq +\pi . \quad (28)$$

One establishes that Eq.(27) are satisfied, by strict analogy with §3.

There remain the periodic boundary conditions,

$$a(m_1, m_2, \dots, m_r) = a(m_2, \dots, m_r, m_1 + N)$$

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$$\begin{aligned}
 & \sum_P \exp i \left( \sum_{k=1}^r f_{P_k} m_k + (1/2) \sum_{k < n} \varphi_{P_k, P_n} \right) \\
 &= \sum_{P'} \exp i \left( \sum_{k=2}^r f_{P'(k-1)} m_k + f_{P'r}(m_1 + N) + (1/2) \sum_{k < n} \varphi_{P'k, P'n} \right)
 \end{aligned}$$

This holds for all  $m_1, \dots, m_r$ ; therefore terms on the left-hand and right-hand sides of the equation which have the same dependence on  $m_k$  must be precisely equal. For example, consider a term  $P$  on the left and  $P''$  on the right, with  $P''$  defined by

$$P''(k-1) = P_k \quad (k=2, \dots, r), \quad P''r = P_1.$$

There results:

$$\begin{aligned}
 & Nf_{P''r} + (1/2) \sum_{k < n} \varphi_{P''k, P''n} - (1/2) \sum_{k < n} \varphi_{P_k, P_n} = 2\pi\lambda \\
 &= Nf_{P_1} + (1/2) \sum_{k < n \leq r-1} \varphi_{P(k+1), P(n+1)} + (1/2) \sum_{k=1}^{r-1} \varphi_{P(k+1), P_1} - (1/2) \sum_{2 \leq k < n} \varphi_{P_k, P_n} \\
 & \quad - (1/2) \sum_{k=2}^r \varphi_{P_1, P_k} \\
 &= Nf_{P_1} - \sum_{k=2}^r \varphi_{P_1, P_k}
 \end{aligned}$$

making use of  $\varphi_{kn} = -\varphi_{nk}$ . Since this relation holds for every  $P$ , it follows that

$$Nf_i = 2\pi\lambda_i + \sum_{k \neq i} \varphi_{ik} \quad (29)$$

for all  $i=1, \dots, r$ .

In complete analogy with §3, one further can show that two  $f_j$ 's can never coincide, otherwise all the coefficients vanish, and therefore for real  $f_j$  two succeeding  $\lambda_j$ 's must differ by at least 2. The number of solutions with real  $f$ 's is thus:

$$\binom{N-r-1}{r} \text{, far fewer than } \binom{N}{r}.$$

the number of solutions we seek.

§6. If  $f_k = u_k + iv_k$  is a complex wave number, then it follows from

$$Nf_k = 2\pi\lambda_k + \sum_{n \neq k} \varphi_{kn}$$

that at least one of the  $\varphi_{kn}$ 's has to have a very large imaginary part of  $O(N)$ . That means in first approximation (cf. §4.)

$$2 \cot \varphi_{kn}/2 = \cot f_k/2 - \cot f_n/2 = -2i.$$

That is, there must be an  $f_n$  such that the real part of  $\cot(f_n/2)$  must agree with that of  $\cot(f_k/2)$ , while their imaginary parts differ by 2 (to  $O(e^{-N})$ ). One is led to the following solution, which we shall denote a *wavecomplex* [Editor's note: a many-spin bound state, i.e. a *soliton*]:

$n$  wave numbers are defined by the equations:

$$\cot f_x/2 = a - ix ; x = -(n-1), -(n-3), \dots, +(n-1) \quad (30)$$

in which  $a$  is a constant for all  $n$  wave numbers. Clearly,

$$\varphi_{x,x \pm 2} = \psi - (\pm)i\infty$$

where the remaining  $\varphi$ 's have finite imaginary parts.  $\psi$  remains undetermined. Applying (15) one obtains

$$\sin u_x / [\cosh v_x - \cos u_x] = a, \quad \sinh v_x / [\cosh v_x - \cos u_x] = x,$$

for which the solutions are:

$$u_x = \tan^{-1} 2a/(a^2+x^2-1) = \tan^{-1} a/(x+1) - \tan^{-1} a/(x-1),$$

$$\tanh v_x = 2x/(a^2+x^2-1) \quad (31)$$

$$e^{2v_x} = [(x+1)^2+a^2]/[(x-1)^2+a^2] \quad (32)$$

and  $\sin u$  has therefore the sign of  $a$ .

We assert that  $a$  can be expressed using the total wave number of our wavecomplex,

$$k = \sum_{x=-(n-1)}^{n-1} f_x = \sum_x u_x \quad (33)$$

which, in simplest form, is

$$a = n \cot k/2 . \quad (34)$$

For  $n=1$  this is evident, for  $n=2$  it follows by inserting the solution obtained earlier (Eq.(18), §4):

$$e^{-v} = \cos u, u = k/2 \text{ (or } k/2 + \pi\text{)},$$

$$a = \sin u / [\cosh v - \cos u] = -\sin u / [(1/2)((\cos u)^{-1} + \cos u) - \cos u]$$

$$= 2 \cot u = 2 \cot k/2 .$$

On the other hand, at fixed  $a$ , the wave numbers for a complex of  $n$  waves are exactly the same as for a complex of only  $n-2$  waves, there are only two new wave numbers  $u_{n-1} = u_{-(n-1)}$  to be added, so that

$$(1/2)k_n = (1/2)k_{n-2} + u_{n-1} . \quad (33a)$$

Now taking (34) for  $n-2$  as proven, then

$$\begin{aligned} (1/2)k_n &= \cot^{-1} a/(n-2) + \cot^{-1} (a/n) - \cot^{-1} a/(n-2) \\ &= \cot^{-1} (a/n) \end{aligned}$$

We further assert that our wavecomplex has eigenvalue

$$\epsilon_n = (1/n) (1 - \cos k) . \quad (35)$$

This is also evident for  $n=1$ , and for  $n=2$  proved in (19). In general,

$$\begin{aligned}
 \epsilon_n &= \sum_{k=-(n-1)}^{n-1} (1 - \cos(u_k - iv_k)) = \epsilon_{n-2} + 2 - \cos(u_{n-1} + iv_{n-1}) - \cos(u_{n-1} - iv_{n-1}) \\
 &= \epsilon_{n-2} + 2(1 - \cos u_{n-1} \cosh v_{n-1}) \\
 &= \epsilon_{n-2} + 2\left(1 - \frac{[a^2+(n-1)^2-1][a^2+(n-1)^2+1]}{[a^2+(n-1)^2+1]^2 - 4(n-1)^2}\right) \\
 &= \epsilon_{n-2} + 4 \frac{a^2 - n(n-2)}{(a^2+n^2)(a^2+(n-2)^2)}
 \end{aligned}$$

using (31), (32). We now assume (35) to be valid for  $n-2$  and use (34), from which it follows that

$$\begin{aligned}
 (1/2)\epsilon_n &= \frac{1}{(n-2)(1 + a^2/(n-2)^2)} + 2 \frac{a^2 - n(n-2)}{(a^2+n^2)(a^2+(n-2)^2)} \\
 &= \frac{(n-2)(a^2+n^2) + 2(a^2-n(n-2))}{(a^2+n^2)(a^2+(n-2)^2)} \\
 &= \frac{n}{a^2 + n^2} = \frac{1}{n} (1 - \cos k).
 \end{aligned}$$

Finally, by analogy with §4, we establish the following: if the number of right-handed spins  $r$  and the total wave number  $k$  of all spin waves is given, then one obtains the smallest eigenvalue  $\epsilon$  when one combines all  $r$  spin waves into a single wavecomplex of eigenvalue  $\epsilon_r = (1/r)(1 - \cos k)$ . For if one has two wavecomplexes with  $n$  and  $p = r - n$  waves, then  $\epsilon_{p+n} = (1/n)(1 - \cos k_1) + (1/p)(1 - \cos(k - k_1))$ . The minimum of this expression is at  $(1/n) \sin k_1 = (1/p) \sin(k - k_1)$ ,  $\sin k_1 = n \sin k / \sqrt{(n^2 + 2np \cos k + p^2)}$ , and is:  $\epsilon_{\min} = (1/np)[n+p - \sqrt{(n^2 + 2np \cos k + p^2)}]$ . Certainly,  $(n+p) \sqrt{(n^2 + 2np \cos k + p^2)} < (n+p)^2 - np(1 - \cos k)$ , as immediately seen by squaring both sides. From this it follows directly that

$$\epsilon_r < \epsilon_{\min} \quad (36)$$

If the spin waves are composed of more than two wavecomplexes, naturally  $\epsilon$  is still larger. The state of lowest energy for  $r$  right-handed spins is then, for  $J > 0$  (ferromagnetic case,) a single wave complex of  $r$  spins; or, if  $J < 0$  (the more usual case,)  $r$  individual waves with real wave numbers. In the latter instance, of course, the lowest energy state has not yet been fixed by this expedient.

It is easy to compute the second approximation for the wave numbers in a wavecomplex, by using the  $\nu$  and  $\nu'$  of formulas (31),(32), altering them slightly in order to satisfy the actual periodic boundary conditions (29). The solution proceeds analogously to §4; one finds that in general for finite  $k$  one solution in the immediate vicinity of (31),(32) is allowed, while for small  $k$  of  $O(1/\sqrt{N})$ , the nature of the solution changes if  $Nk/2\pi = \lambda$  is indivisible by  $n$ . Instead of a complex of three spin waves there would occur, for example, a pair of conjugate complex waves as were already analyzed in §4 for even  $\lambda$ , together with a single wave of almost the same, but real, wave number. The number of solutions is unaffected by this change of appearance. There is one solution for  $\lambda=0,1,2,\dots,N-n$ ; the last value corresponds to  $\lambda-(n-1)=\lambda-(n-3)=\dots=\lambda_{n-1}=N-1$ . For  $\lambda > N-n$ , one or more  $\lambda_k$  would =  $N$ , which is not allowed.

From now on we shall also exclude  $\lambda_i = 0$  in general. We immediately gain in symmetry from this, and automatically distinguish those solutions for which the left-handed component of total spin  $M = (1/2)N - r = S_{\text{tot}}$ , the total spin, from all those others with the same value of  $M$  which belong to a higher value of  $S_{\text{tot}}$ . The latter are just those states in which one or more of the  $r$  wave numbers are zero. After eliminating them, there remain only  $N-2n+1$  wavecomplex solutions of  $n$  spin waves:  $\lambda=n,n+1,\dots,N-n$ .

§7. We assume that two complexes of  $n$  and of  $p$  ( $>n$ ) spin waves are available, and ask about the number of solutions that can be obtained by means of the ansatz. This requires we discuss the phases  $\psi$ . If the wave numbers in the first complex are given by

$$\cot f_X/2 = a - ix, \quad x = -(n-1), (n-3), \dots n-1 \\ a = n \cot k_1/2, \quad k_1 = \sum_X f_X \quad (37a)$$

and in the second by

$$\cot f_\mu/2 = b - i\mu, \quad \mu = -(p-1), (p-3), \dots p-1 \\ b = p \cot k_2/2, \quad k_2 = \sum_\mu f_\mu \quad (37b)$$

then by (28),(29),(31)

$$\begin{aligned} Nk_1 &= 2\pi\lambda_1 + \sum_X \sum_\mu \psi_{X,\mu} \\ Nk_2 &= 2\pi\lambda_2 - \sum_X \sum_\mu \psi_{X,\mu} \end{aligned} \quad \left. \right\} \quad (38)$$

$$\cot \psi_{X,\mu} = \cot (\psi_{X,\mu} + i\chi_{X,\mu}) = (1/2)(a-b) - (i/2)(x-\mu) \\ \tan \psi_{X,\mu} = (a-b)/[(1/4)(a-b)^2 + (1/4)(x-\mu)^2 - 1]$$

The sign of  $\psi_{X,\mu}$  = sign of  $a-b$ , and  $\sum_X \sum_\mu \chi_{X,\mu} = 0$ , because the  $f_X$  and  $f_\mu$  come in ordered complex conjugate pairs.

The  $\psi_{X,\mu}$  are zero if  $k_1$  is very small,  $a$  very large, and then with increasing  $k_1$  they become positive as long as  $a > b$ . We are interested most of all in their value for the case where  $a$  approaches  $b$  very closely and ultimately becomes smaller than  $b$ , in order to determine the number of forbidden integers  $\lambda_1, \lambda_2$ . For this we fix<sup>10</sup>  $\lambda_0 = Nk_2/2\pi$  and define  $\lambda'$  through

$$n \cot \pi\lambda'/N > p \cot \pi\lambda_0/N > n \cot \pi(\lambda'+1)/N \quad (39)$$

---

<sup>10</sup> We shall see later that for  $a \approx b$ ,  $k_1$  and  $k_2$  in fact have the form  $2\pi/N \times$  integer, and that therefore  $\lambda_0 = \text{integer}$

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For  $Nk_1 = 2\pi\lambda'$ ,  $a-b$  will evidently be positive and small, of  $O(1/N)$ . Then,  $\tan \psi_{x,\mu}$  is small and positive if  $|x-\mu| > 2$ ; small and negative if  $|x-\mu| < 2$  and very large and positive if  $|x-\mu| \approx 2$ .

The last is a consequence of the  $x$  and  $\mu$  differing from integers only by quantities  $O(e^{-N}) \ll 1/N^2$  (cf. §4), such that  $(1/4)(x-\mu)^2 - 1 \ll (a-b)^2$  as soon as  $|x-\mu|$  lies in the vicinity of 2. Up to quantities  $O(1/N)$ :

$$\psi_{x,\mu} = \begin{cases} 0 & \text{for } |x-\mu| > 2 \\ \pi & \text{for } |x-\mu| < 2 \\ \pi/2 & \text{for } |x-\mu| = 2 \end{cases} \quad (40)$$

Next, assume  $p-n$  is odd.

Then for a given  $x$  there are just two values  $\mu=x+1$  and  $\mu=x-1$  for which  $\psi_{x,\mu}$  does not vanish, but has the value  $\pi$ . This yields

$$\sum_x \sum_\mu \psi_{x,\mu} = 2\pi n . \quad (41)$$

$p-n$  is even.

For each  $x$  there are 3  $\mu$ 's for which  $\psi_{x,\mu} \neq 0$ :

$$\begin{array}{ll} \mu=x, & \psi_{x,\mu} = \pi \\ \mu=x+2, & \psi_{x,\mu} = \pi/2 \\ \mu=x-2, & \psi_{x,\mu} = \pi/2 . \end{array}$$

Together, this yields once again  $\sum_x \sum_\mu \psi_{x,\mu} = 2\pi n .$

So,

$$\lambda_1 = Nk_1/2\pi - n = \lambda' - n \quad \text{and} \quad \lambda_2 = \lambda_0 + n . \quad (42a)$$

Correspondingly for  $Nk_1 = 2\pi(\lambda'+1)$ :

$$\sum_x \sum_\mu \psi_{x,\mu} = -2\pi n , \quad \lambda_1 = \lambda' + 1 + n , \quad \text{and} \quad \lambda_2 = \lambda_0 - n . \quad (42b)$$

Thus  $\lambda_1$  ranges over the values,

$$\lambda_1 = n, N+1, \dots, \lambda'-n, \lambda' + n+1, \dots, N-n . \quad (42c)$$

The  $2n$  values  $\lambda'-n+1, \dots, \lambda'+n$  are forbidden by the presence of the other spin complexes. Thus, we see that if  $\lambda_0$  is small, then in general  $b > a$ , thus  $\lambda_2 = \lambda_0 - n$ . However,  $\lambda_2$  must be at least equal to  $p$  (see end of preceding paragraph) and therefore,  $\lambda_0 \geq p+n$ . Likewise  $\lambda_0 \leq N-p-n$ , from which it follows that  $\lambda_0$  can take on exactly  $N-2n-2p+1$  values. This is again  $2n$  fewer than if the other spin complex were not present. It is important in both cases that  $n$  be the number of waves of the *smaller* of the two spin complexes. The total number of solutions is, then,

$$(N - 2n - 2p + 1) \times (N - 4n + 1).$$

The case  $n=p$  remains to be investigated. Here for  $x=n-1$ , the single partner,  $\mu=x+2$ , which earlier gave  $\psi_{x,\mu} = \pi/2$ , is missing, and for  $x=-(n-1)$ , the partner  $\mu=x-2$  is missing, so now

$$\sum_x \sum_\mu \psi_{x,\mu} = -(2n-1)\pi . \quad (43)$$

In addition, there is now a  $\lambda'$ , so that  $ncot \pi\lambda'/N = pcot \pi\lambda_0/N$  and, simply,  $\lambda' = \lambda_0$ . But this does not lead to a solution because whenever  $f_x = f_\mu$ ,  $x = \mu$ , and the eigenfunction has already been seen to vanish if two wave numbers are equal. That is,  $k_1$  is at most  $Nk_1 = 2\pi(\lambda_0 + 1)$ , which yields

$$\lambda_1 = \lambda_0 - 1/2 - n \quad \text{and} \quad \lambda_2 = \lambda_0 - 1/2 + n ;$$

just as, for  $Nk_1 = 2\pi(\lambda_0 + 1)$ ,

$$\sum_x \sum_\mu \psi_{x,\mu} = -(2n-1)\pi \quad \text{and} \quad \lambda_1 = \lambda_0 + 1/2 + n, \quad \lambda_2 = \lambda_0 + 1/2 - n .$$

$\lambda_0$  is therefore, obviously, a half integer. Over the range of  $\lambda_1$ , once again  $2n$  numbers are missing:  $\lambda_0 - n + 1/2, \dots, \lambda_0 + n - 1/2$ , but only  $2n-1$  in the range of  $\lambda_0$ , so  $\lambda_0$  must equal or exceed  $2n-1/2$  ( $\lambda_2 = n$ ), while it is at most equal to

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$N-2n+1/2$  ( $\lambda_2=N-3n+1$ ), that is,  $\lambda_0$  possesses  $N-4n+2$  values instead of the  $N-2n+1$  which are allowed when only a single complex of  $n$  waves is present. As interchange of  $\lambda_1$  and  $\lambda_2$  does not affect the solution, the total number of solutions is  $(1/2)(N-4n+2) \times (N-4n+1)$ .

The situation will perhaps become clearer if, for the moment, we normalized the  $\psi$  differently. Let  $\psi'$  be defined such that, for very large  $a$  it coincides with  $a$ , but for  $a=b$  it remains constant. Then (in the case of two complexes with  $n$  waves,)  $\sum_K \sum_\mu \psi'_{K,\mu}$  grows from zero to  $(2n-1)2\pi$ , while  $k_1$ , with  $k_2$  fixed, goes from  $2\pi n/N$  to  $2\pi(N-n)/N$ .

If  $2\pi\lambda_1' = Nk_1 - \sum_K \sum_\mu \psi'_{K,\mu}$ , then  $\lambda_1'$  clearly takes on all values from  $n$  to  $N-3n+1$ , that is  $N-4n+2$  values; this also applies to  $\lambda_2$ , with the one restriction, a prohibition against the value which corresponds to  $k_2=k_1$ .

Now, in general we assume  $q_n$  complexes each with  $n$  waves, that is:  $q_1$  single waves with real wave numbers,  $q_2$  pairs with complex conjugate wave numbers, and so on. The constant  $\lambda_1$  of the first of the  $n$  wave complexes could assume any of the values  $n, n+1, \dots, N-n$ , i.e. take on  $N-2n+1$  possible values if there were no other wavecomplex present. For each complex with  $p > n$  waves,  $2n$  numbers are lost, as we have seen; for each complex of  $p < n$ , only  $2p$ ; finally, for each of the remaining  $q_n-1$  complexes with  $n$  waves,  $2n-1$  numbers. Thus, there are

$$Q_n' = N-2n+1 - 2\sum_{p<n} pq_p - 2\sum_{p>n} nq_p - (2n-1)(q_n-1)$$

remaining values allowed for  $\lambda_1$ . The constant  $\lambda_2$  of the second complex of  $n$  waves may not allow  $k_2$  to coincide with  $k_1$ , that is, it has one fewer possibilities; finally, the constant  $\lambda_{q_n}$  of the last complex of  $n$  waves can take on only

$$Q_n' - (q_n-1) = Q_n + 1$$

distinct values, where

$$Q_n(N, q_1, q_2, \dots) = N - 2\sum_{p < n} p q_p - 2\sum_{p \geq n} n q_p \quad (44)$$

Finally, considering that interchange of the  $\lambda$ 's of the various wavecomplexes with equal numbers of waves  $n$  does not lead to new solutions, one finds for the total number of solutions

$$z(N, q_1, q_2, \dots) = \prod_{n=1}^{\infty} \frac{(Q_n + q_n) \cdots (Q_n + 1)}{q_n!} = \prod_n \left( \frac{Q_n + q_n}{q_n} \right) \quad (45)$$

where the  $Q_n$  are defined by (44).

§8. We shall prove now that we have obtained the correct number of solutions. It is known that the number of eigenvalues  $z(N, r)$  for a fixed value of total spin  $S_{\text{tot}} = N/2 - r$  equals the number of eigenvalues with  $M = S_{\text{tot}}$  left-handed spins, less the number for  $M = S_{\text{tot}} + 1$ , i.e.!

$$z(N, r) = \binom{N}{r} - \binom{N}{r-1} = \frac{N-2r+1}{N-r+1} \times \binom{N}{r} \quad (46)$$

The following must also hold true:

$$\sum_{q_1, q_2, \dots} z(N, q_1, q_2, \dots) = z(N, r) \quad (47)$$

the sums being over all values spanned by  $q_1, q_2, \dots$  for which the total number of spin waves equals  $r$ , that is

$$q_1 + 2q_2 + 3q_3 + \dots = \sum n q_n = r.$$

In other words, one sums over the "partitio numerorum" of  $r$ :  $q_n$  gives the number of times the summand  $n$  appears in the particular partition.

We introduce the *total index* of the spin complex:

$$q = \sum_n q_n \quad (48)$$

and rewrite (44) as:

$$\begin{aligned} Q_n(N, q_1 q_2 \dots) &= N - 2q - 2 \sum_{p < n} (p-1) q_p - 2 \sum_{p \geq n} (n-1) q_p \\ &= Q_{n-1}(N - 2q, q_2 q_3 \dots). \end{aligned} \quad (49)$$

A special case:

$$Q_1(N, q_1 q_2 \dots) = N - 2q. \quad (49a)$$

Using this in (45),

$$z(N, q_1 q_2 \dots) = \binom{N-2q+q_1}{q_1} \cdot z(N-2q, q_2 q_3 \dots). \quad (50)$$

On the right, next to the binomial coefficient, is the number of allowed solutions with  $q_2$  single spin waves, and generally,  $q_n$  complexes each with  $n-1$  waves in a chain of  $N-2q$  sites. This corresponds to a total of

$$r' = \sum_n q_n (n-1) = r-q \quad (50a)$$

right-handed spins arranged in

$$q' = \sum_{n \geq 2} q_n = q-q_1 \quad (50b)$$

wavecomplexes. Now we introduce the number of all these solutions, for which  $r$  right-handed spins are arranged in precisely  $q$  wavecomplexes, without distinguishing how many waves each individual complex contains:

$$z(N, r, q) = \sum_{\substack{q_1 + q_2 + q_3 + \dots = q \\ q_1 + 2q_2 + 3q_3 + \dots = r}} z(N, q_1 q_2 \dots) \quad (51)$$

It follows then from (50), (50a), (50b) that

$$z(N, r, q) = \sum_{q_1=0}^{q-1} \binom{N-2q+q_1}{2q_1} z(N-2q, r-q, q-q_1) \quad (52)$$

and

$$z(N,r) = \sum_{q_1=0}^r z(N,r,q_1). \quad (53)$$

From here on we treat the problem by complete induction. We assume

$$z(N,r,q) = \frac{N-2r+1}{N-r+1} \binom{N-r+1}{q} \binom{r-1}{q-1} \quad (54)$$

For  $q=1$  this is certainly correct - we have a single complex of  $r$  waves whose wave numbers can take on  $N-2r+1$  values. Likewise, (54) is correct for  $q=r$ ; then  $q_1=r$  and  $q_{\eta}=0$  for  $\eta>1$  inserted into (45) transforms it into (54). Let us take (54) as proven for  $N-2q, r-q, q-q_1$  and by (52) have

$$z(N,r,q) = \sum_{q_1=0}^{q-1} \binom{N-2q+q_1}{q_1} \binom{N-r-q+1}{q-q_1} \binom{r-q-1}{q-q_1-1} \frac{N-2r+1}{N-r+1}.$$

Then,

$$\binom{N-2q+q_1}{q_1} = \sum_{s=0}^{q_1} \binom{r-1}{s} \binom{N-2q+q_1+1-r}{q_1-s}$$

$$z(N,r,q) = \sum_{q_1=0}^{q-1} \sum_{s=0}^{q_1} \frac{(N-r-q+1)!}{(q-q_1)!(N-r-2q+q_1+1)!} \frac{(N-r-2q+q_1+1)!}{(q_1-s)!(N-r-2q+s+1)!} \frac{N-2r+1}{N-r-q+1}$$

$$\times \binom{r-1}{s} \binom{r-q-1}{q-q_1-1},$$

$$= \frac{N-2r+1}{N-r-q+1} \sum_{s=0}^{q-1} \binom{r-1}{s} \binom{N-r-q+1}{q-s} \sum_{q_1=s}^{q-1} \binom{q-s}{q_1-s} \binom{r-q-1}{q-q_1-1}$$

$$= \frac{N-2r+1}{N-r-q+1} \sum_s \binom{N-r-q+1}{q-s} \frac{(r-1)!}{s!(r-s-1)!} \frac{(r-s-1)!}{(q-s-1)!(r-q)!}$$

$$= \frac{N-2r+1}{N-r-q+1} \binom{r-1}{q-1} \sum_s \binom{q-1}{s} \binom{N-r-q+1}{q-s}$$

$$= \frac{N-2r+1}{N-r-q+1} \binom{r-1}{q-1} \binom{N-r}{q}$$

identical with (54). Since (54) holds for  $q=1$  and for  $q=2, r=2$  — and trivially, also for  $q=2, r=1$  — its validity can be proven for  $q=2, r=3$  and 4, then for  $q=2$  and  $r=3, 4$ , then for  $q=2$  and greater values of  $r$ , and finally for  $q=3, 4$ , etc. Inserting (54) in (53) yields:

$$z(N,r) = \frac{N-2r+1}{N-r+1} \sum_{q=1}^r \binom{r-1}{r-q} \binom{N-r+1}{q} = \frac{N-2r+1}{N-r+1} \binom{N}{r}$$

in agreement with the number of solutions which we were seeking, Eq.(46). *Therefore, our method yields all the solutions of this problem.*

In a future paper, this method will be extended to [three-dimensional] space lattices,<sup>11</sup> and its physical implications for cohesion, ferromagnetism and electrical conductivity, will be derived.

I give my heartfelt thanks to Prof. Fermi for especially numerous and stimulating discussions. Also, I thank the Rockefeller Foundation for the grant of a stipend which made my stay in Rome possible.

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<sup>11</sup> *Ed. note:* this rash promise has apparently not been kept.

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## On the Quantum Theory of the Temperature of Absolute Zero

(with G. Beck and W. Riezler)

*Die Naturwissenschaften* 19, 39 (1931)

This joke was meant to make fun of papers by Eddington in which he claimed to derive the value of the fine structure constant to be  $1/\alpha = \hbar c/e^2 = 137$ . He started from Dirac's theory which uses a  $4 \times 4$  matrix for an electron. Dirac had (erroneously) assumed that a proton is a hole in the, generally filled, sea of negative energy states of the electron, so Eddington assumed there should again be a  $4 \times 4$  matrix pertaining to a proton. For a proton and an electron, the two elementary particles then known and interacting by electric forces, you would then need a  $16 \times 16$  matrix which, if symmetric, has 136 distinct matrix elements. Add one for the orbital motion of the electron around the proton makes 137 "digress of freedom", a number close to the then known value of  $1/\alpha$ . Modern measurements give 137.0360.

Beck, Riezler and I were at Cambridge on fellowships and had listened to Eddington's unbelievable talk about the number 137.

## On the Quantum Theory of the Temperature of Absolute Zero

*Die Naturwissenschaften*, January 9, 1931

Let us consider a hexagonal lattice. The absolute zero of the lattice is characterized by the fact that all degrees of freedom of the system are frozen out, i.e. all inner movements of the lattice have ceased, with the exception, of course, of the motion of an electron in its Bohr orbit. According to Eddington every electron has  $1/\alpha$  degrees of freedom where  $\alpha$  is the fine structure constant of Sommerfeld. Besides electrons our crystal contains only protons and for these the number of degrees of freedom is obviously the same since, according to Dirac, a proton is considered to be a hole in a gas of electrons. Therefore to get to the absolute zero we have to remove from the substance per neutron (= 1 electron plus 1 proton; our crystal is to carry no net charge)  $2/\alpha - 1$  degrees of freedom since one degree of freedom has to remain for the orbital motion. We thus obtain for the zero temperature

$$T_0 = -(2/\alpha - 1) \text{ degrees.}$$

Putting  $T_0 = -273^\circ$ , we obtain for  $1/\alpha$  the value 137 in perfect agreement within the limits of accuracy with the value obtained by totally independent methods. It can be seen very easily that our result is independent of the particular crystal lattice chosen.

G. Beck, H. Bethe, W. Riezler  
Cambridge, 10 December 1930

### “Correction”

*Die Naturwissenschaften*, March 6, 1931

The note by G. Beck, H. Bethe and W. Riezler, published in the January 9 issue of this journal, was not meant to be taken seriously. It was intended to characterize a certain class of papers in theoretical physics of recent years which are purely speculative and based on spurious numerical agreements. In a letter received by the editors from these gentlemen they express regret that the formulation they gave to the idea was suited to produce misunderstanding.

**On the Stopping of Fast Particles and on the Creation  
of Positive Electrons**  
(with W. Heitler)

*Proc. Roy. Soc. London Ser. A* **146**, 83–112 (1934)

The cross section for electron pair creation, and for bremsstrahlung from fast electrons, is derived from the Dirac theory. The effect of screening by atomic electrons is calculated; it is important for high electron energy. The formulae were later well confirmed by experiments with electrons and  $\gamma$ -rays from accelerators. The paper emphasizes that the theory does *not* agree with cosmic ray results: It was later realized that most of the penetrating particles of low ionization in cosmic rays are  $\mu$ -mesons which should radiate far less than electrons.

The calculation is done in Born approximation. The correction required for high atomic number  $Z$  was later calculated by H. A. Bethe and L. C. Maximon (*Phys. Rev.* **93**, 768, 1954); it turned out to be surprisingly small.

ON THE  
STOPPING OF FAST PARTICLES AND ON THE  
CREATION OF POSITIVE ELECTRONS

By  
H. Bethe and W. Heitler

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## *On the Stopping of Fast Particles and on the Creation of Positive Electrons*

By H. BETHE, Manchester, and W. HEITLER, Bristol

(Communicated by P. A. M. Dirac, F.R.S.—Received February 27, 1934)

### *Introduction*

The stopping power of matter for fast particles is at present believed to be due to three different processes : (1) the ionization ; (2) the nuclear scattering ; (3) the emission of radiation under the influence of the electric field of a nucleus. The first two processes have been treated in quantum mechanics by Bethe,<sup>†</sup> Møller,<sup>‡</sup> and Bloch<sup>§</sup> in a very satisfactory way. A provisional estimation of the order of magnitude to be expected in the third process has been given by Heitler.<sup>||</sup> The result obtained was that the cross-section  $\phi$  for the energy loss by radiation for very fast particles (if the primary energy  $E_0 \gg mc^2$ ) is of the order

$$\phi \sim \frac{Z^2}{137} \left( \frac{e^2}{mc^2} \right)^2, \quad (1)$$

where  $Z$  is the nuclear charge.

It is the aim of the present paper to discuss in greater detail the rate of loss of energy by this third process and its dependence on the primary energy ; in particular we shall consider the effect of *screening*. The results obtained for very high energies ( $> 137 mc^2$ ) seem to be in disagreement with experiments made by Anderson (cf. § 7).

By an exactly similar calculation another process can be studied, namely, the "twin birth" of a positive and negative electron due to a light quantum in the presence of a nucleus. This process is the converse of the scattering of an electron with loss of radiation, if the final state has *negative energy*. The results are in exact agreement with recent measurements for  $\gamma$ -rays of  $3-10 mc^2$ . A provisional estimate of the probability of this process has been given by Plesset and Oppenheimer,<sup>¶</sup> who also obtain for the cross-section a quantity of the order of magnitude given by equation (1).

<sup>†</sup> 'Ann. Physik,' vol. 5, p. 325 (1930) ; 'Z. Physik,' vol. 76, p. 293 (1932).

<sup>‡</sup> 'Ann. Physik,' vol. 14, p. 531 (1932).

<sup>§</sup> 'Z. Physik,' vol. 81, p. 363 (1933) ; 'Ann. Physik,' vol. 16, p. 285 (1933).

<sup>||</sup> 'Z. Physik,' vol. 84, p. 145 (1933). Referred to later as I.

<sup>¶</sup> 'Phys. Rev.,' vol. 44, p. 53 (1933).

## I. THEORY

§ 1. *The Cross-section for the Energy-loss by Radiation*

1. *General Method.*—In order to obtain the rate of loss of energy of a particle by emission of radiation, we have to calculate the transition probability for the following process : a particle with momentum†  $p_0/c$  and energy  $E_0$  makes a transition to a state with the momentum  $p/c$  and energy  $E$ , while a light quantum with the momentum  $k/c$  is emitted, the frequency  $\nu$  being given by

$$k = \hbar\nu = E_0 - E. \quad (2)$$

The perturbation causing this transition is the interaction of the particle with the nuclear field  $V = Ze^2/r$  and with the radiation field  $H = -e(\alpha A)$ , where  $A$  is the vector potential of the radiation field and  $\alpha$  is Dirac's three-dimensional matrix-vector signifying the velocity.

The wave functions of the electron describing the initial and the final state are supposed to be plane waves, the atomic field being only considered as a perturbation. This corresponds to the first approximation of Born's collision theory, which was shown by Bethe (*loc. cit.*) to hold for  $Z/137 < v/c$ . For fast particles ( $v \approx c$ ) this is always true, if  $Z$  is not too large. For lead, however, it is doubtful whether the calculations give quantitatively correct results. But from the experiments it seems that, at least for the twin birth, see § 8, the error is very small.

The transition from the initial to the final state, however, only occurs under the simultaneous action of both the atomic field and that of the light wave. First, the electron goes, under the influence of one of the said perturbations, from the initial state to an intermediate state (conservation of energy does not necessarily hold here); then a second transition immediately happens to the final state, caused by the other perturbation. Since momentum is conserved in the emission of light, it can easily be seen (*cf. I*) that there exist two such intermediate states, where the electron has a momentum  $p'$ ,  $p''$  (energies  $E'$ ,  $E''$ ) given by :

$$\begin{aligned} \text{I} \quad p' &= p + k & \text{no light quantum present } \} \\ \text{II} \quad p'' &= p_0 - k & \text{a light quantum } k \text{ present } \} \end{aligned} \quad (3)$$

† It is convenient to express the momentum in energy units  $p = c \times$  momentum. Throughout the rest of the paper we shall speak freely of  $p$  as the momentum instead of the strictly more correct  $p/c$ .

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If we denote the initial state (momentum  $\mathbf{p}_0$ , no light quantum) by A, and the final state (momentum  $\mathbf{p}$ ,  $\mathbf{k}$ ) by E, the transition probability per unit time becomes (see I, equation (27))

$$w = \frac{2\pi}{\hbar} \rho_E \rho_k dk \left| \sum \frac{H_{EI} V_{IA}}{E' - E_0} + \sum \frac{V_{EI} H_{IA}}{E'' - E} \right|^2, \quad (4)$$

where  $\rho_E$ ,  $\rho_k$  are the numbers of quantum states per unit volume, per unit solid angle and per unit energy interval for the electron and the light quantum in the final state; so that

$$\rho_E dE = \frac{\Omega_E p E dE}{h^3 c^3}, \quad \rho_k dk = \frac{\Omega_k k^2 dk}{h^3 c^3}, \quad (5)$$

( $\Omega_E$ ,  $\Omega_k$  being the elements of the solid angle).

The wave functions that occur in the matrix elements in (5) are normalized in such a way that there is one particle per unit volume. The summation in (4) has to be extended over both the spin directions and both signs of the energy of the intermediate states.

To obtain the differential cross-section from (4), we have, according to our method of normalization, to divide by the velocity of the incident electron,  $v_0 = cp_0/E_0$ . Putting in the values for the matrix elements for a pure Coulomb field (cf. I equations (18)-(21)) we obtain the differential cross-section

$$d\Phi = \frac{Z^2 e^4}{137\pi^2} \frac{\Omega_E \Omega_k p E E_0 k dk}{p_0 c^4} \left| \sum \frac{(u^* \alpha_k u') (u'^* u_0)}{E' - E_0} + \sum \frac{(u^* u'') (u''^* \alpha_k u_0)}{E'' - E} \right|^2, \quad (6)$$

where

$$\mathbf{q} = \mathbf{p}_0 - \mathbf{p} - \mathbf{k}, \quad (7)$$

denotes the momentum transferred to the nucleus in the process.  $u$ ,  $u'$  are the amplitudes of the plane waves with momenta  $\mathbf{p}$ ,  $\mathbf{p}'$  each having four components.  $u$  refers to a definite spin direction.  $\alpha_k$  is the component of  $\alpha$  in the direction of the polarization of the light quantum.  $(u^* \alpha_k u') (u'^* u_0)$  depends only upon the angles in terms of which it can easily be expressed. This can be done by the usual method†: first, we carry out the summation  $\Sigma$  over the spin directions and both signs of the energy of the intermediate states (*i.e.*, over all four states having the same momentum  $\mathbf{p}'$ ):

$$\Sigma \frac{(u^* \alpha_k u') (u'^* u_0)}{E_0 - E'} = \frac{E_0 \Sigma (u^* \alpha_k u') (u'^* u_0)}{E_0^2 - E'^2} + \frac{\Sigma (u^* \alpha_k E' u') (u'^* u_0)}{E_0^2 - E'^2}.$$

In the first term we have simply (Vollständigkeitsrelation)

$$\Sigma (u^* \alpha_k u') (u'^* O u_0) = (u^* \alpha_k u_0). \quad (8)$$

† Casimir, 'Helv. Phys. Act.', vol. 6, p. 287 (1933).

For the second we use the wave equation

$$E'u' = [(\alpha p') + \beta \mu] u' \equiv H'u',$$

where  $\mu = mc^2$ . This equation holds for both signs of  $E'$ , since the operator  $H'$  is independent of the sign of  $E'$ . Hence

$$\Sigma (u^* \alpha_k E' u') (u'^* u_0) = \Sigma (u^* \alpha_k H' u') (u'^* u_0) = (u^* \alpha_k H' u_0). \quad (9)$$

And finally

$$\Sigma \frac{(u^* \alpha_k u') (u'^* u_0)}{E_0 - E'} = \frac{E_0 (u^* \alpha u_0) + (u^* \alpha_k H' u_0)}{E_0^2 - E'^2}. \quad (10)$$

(10) holds for definite spin directions of the initial and the final states. As we are not interested in the probability for special spin directions, we sum also over the spin directions of the final state. Using equation (10) we obtain then from (6) expressions of the form

$$S (u^* {}_0 A u) (u^* B u_0),$$

where the summation  $S$  has to be taken over the spin directions of the final state only, but not over the two signs of the energy. But this sum  $S$  can be reduced to a sum  $\Sigma$  over all four states of both spin and energy. For we have

$$Eu = Hu, \quad \text{or} \quad u = \frac{H + E}{2E} u. \quad (11)$$

For the states of *negative energy* with the wave function  $\tilde{u}$  the expression  $(H + E)\tilde{u}$  vanishes. Introducing the operator  $(H + E)u/2E$  instead of  $u$ , we may now extend the summation also over both signs of the energy, obtaining

$$S (u^* {}_0 A u) (u^* B u_0) = \Sigma \left( u^* {}_0 A \frac{H + E}{2E} u \right) (u^* B u_0) = \left( u^* {}_0 A \frac{H + E}{2E} B u_0 \right). \quad (12)$$

(12) is the average value of the operator  $A(H + E)/2EB$  in the initial state. It can be evaluated by the usual methods.

2. *Differential and Integral Cross-sections*.—If one applies this method to (6) one can easily obtain the differential cross-section

$$\begin{aligned} d\Phi = & \frac{Z^2 e^4}{137 \cdot 2\pi} \frac{dk}{k} \frac{p}{p_0} \frac{\sin \theta \sin \theta_0 d\theta d\theta_0 d\phi}{q^4} \int \frac{p^2 \sin^2 \theta}{((E - p \cos \theta)^2 - q^2)} (4E_0^2 - q^2) \\ & + \frac{p_0^2 \sin^2 \theta_0}{(E_0 - p_0 \cos \theta_0)^2} (4E^2 - q^2) - \frac{2p_0 p \sin \theta \sin \theta_0 \cos \phi}{(E - p \cos \theta)(E_0 - p_0 \cos \theta_0)} (4E_0 E - q^2) \\ & + \frac{2k^2 (p^2 \sin^2 \theta + p_0^2 \sin^2 \theta_0 - 2pp_0 \sin \theta \sin \theta_0 \cos \phi)}{(E - p \cos \theta)(E_0 - p_0 \cos \theta_0)}. \end{aligned} \quad (13)$$

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$\theta, \theta_0$  are the angles between  $\mathbf{k}$  and  $\mathbf{p}, \mathbf{p}_0$  respectively,  $\phi$  the angle between the  $(\mathbf{pk})$  plane and the  $(\mathbf{p}_0\mathbf{k})$  plane. The denominators arise from the resonance denominators

$$\left. \begin{aligned} E'^2 - E_0^2 &= (\mathbf{p} + \mathbf{k})^2 - \mathbf{p}_0^2 = -2k(E - p \cos \theta) \\ E''^2 - E^2 &= (\mathbf{p}_0 - \mathbf{k})^2 - \mathbf{p}^2 = 2k(E_0 - p_0 \cos \theta_0) \end{aligned} \right\}. \quad (14)$$

In (14) the summation has already been taken over the directions of polarization, and the spin of the electron in the final state.

In order to obtain the total probability for the emission of a light-quantum of a given frequency  $\nu$ , one has to integrate (14) over the angles, both of the electron and of the light quantum. This integration is elementary but rather tedious. We shall give only the result.<sup>†</sup>

$$\Phi = \frac{Z^2}{137} \left( \frac{e^2}{mc^2} \right)^2 \frac{p}{p_0} \frac{dk}{k} \left\{ \frac{1}{3} - 2E_0 E \frac{p^2 + p_0^2}{p^2 p_0^2} + \mu^2 \left( \frac{\epsilon_0 E}{p_0^3} + \frac{\epsilon E_0}{p^3} - \frac{\epsilon \epsilon_0}{pp_0} \right) + \left[ \frac{8}{3} \frac{E_0 E}{p_0 p} + \frac{k^2}{p_0^3 p^3} (E_0^2 E^2 + p_0^2 p^2) \right] \cdot \log + \frac{\mu^2 k}{2pp_0} \left[ \frac{E_0 E + p_0^2}{p_0^3} \epsilon_0 - \frac{E_0 E + p^2}{p^3} \epsilon + \frac{2k E_0 E}{p^2 p_0^2} \right] \log \right\}, \quad (15)$$

with

$$\left. \begin{aligned} \mu &= mc^2, & \epsilon &= \log \frac{E + p}{E - p} = 2 \log \frac{E + p}{\mu}, \\ \epsilon_0 &= \log \frac{E_0 + p_0}{E_0 - p_0} = 2 \log \frac{E_0 + p_0}{\mu}, \\ \log &= \log \frac{p_0^2 + p_0 p - E_0 k}{p_0^2 - p_0 p - E_0 k} = 2 \log \frac{E_0 E + p_0 p - \mu^2}{\mu k} \end{aligned} \right\}. \quad (15A)$$

For energies large compared with  $mc^2$ , i.e., for

$$E_0 \gg mc^2, \quad E \gg mc^2, \quad k \gg mc^2,$$

(15) reduces to

$$\Phi = \frac{Z^2}{137} \left( \frac{e^2}{mc^2} \right)^2 \frac{dk}{k} \frac{4}{E_0^2} (E_0^2 + E^2 - \frac{2}{3} E_0 E) \left( \log \frac{2E_0 E}{k\mu} - \frac{1}{2} \right). \quad (16)$$

The result will be discussed in § 5, 6, and 7.

<sup>†</sup> The same formulae (13), (15), have been obtained by F. Sauter. We are indebted very much to Dr. Sauter for the communication of his results. The comparison with his results has made it possible to avoid some mistakes in the calculations. The same formula has also been obtained by G. Racah. We wish to thank him also for sending us his results.

### § 2. Creation of Positive Electrons

The creation of a pair of electrons of opposite charge is considered as a kind of photoelectric process: an electron which is initially in a state of negative energy  $E = -|E|$  is excited by a light quantum  $h\nu$  to a state of positive energy

$$E_0 = h\nu - |E|.$$

Then it is observed that a negative electron of energy  $E_0$  and a positive one of energy  $E_+ = |E|$  are created, the light quantum being absorbed.

The reverse of this process would be the transition of an electron from the state  $E_0$  to a state of negative energy, the energy  $E_0 + |E|$  being radiated. This reverse process will not usually occur because the states of negative energy are occupied.<sup>†</sup> The process is identical with that treated in § 1, the only difference being the sign of the final energy. It is clear that this cannot make any difference in the calculation up to formula (10). One might, however, expect a different value for the quantities  $(u^* \alpha_k u_0)$  and  $(u^* \alpha_k H' u_0)$ .

That this is not so can easily be seen from Casimir's method of evaluating quantities of this kind, which has been used already in § 1, equations (8)–(13). If the momentum  $p$  is given, all considerations leading to (13) remain unchanged, except that we have for the wave amplitude  $\tilde{u}$  of a *negative energy state*, instead of (11):

$$\frac{H - |E|}{-2|E|} \tilde{u} = \tilde{u},$$

while for a state of positive energy  $(H - |E|) u = 0$ . Therefore, in (13) nothing is changed except the sign of the energy, viz.,

$$S(u^* {}_0 A \tilde{u}) (\tilde{u}^* B u_0) = \left( u^* {}_0 A \frac{H - |E|}{-2|E|} B u_0 \right) = \left( u^* {}_0 A \frac{H + E}{2E} B u_0 \right). \quad (17)$$

We conclude that formula (13) holds for the reverse process of the creation of pairs as well as for the "normal" emission of radiation. To calculate the probability of the creation itself, one has only to consider that now there exist *two* electrons in the final state instead of one electron and one light quantum. Instead of  $\rho, d\nu$ , we must therefore write in (5)

$$\rho_{E_0} dE_0 = \frac{\Omega_0 E_0 p_0 dE_0}{h^3 c^3},$$

i.e., the number of electronic states with energy between  $E_0$  and  $E_0 + dE_0$

<sup>†</sup> It may happen that a positive electron is annihilated in this way by an inner electron of a heavy atom.

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per unit volume and per solid angle  $\Omega_0$ . Furthermore, one has to divide by the number of incident light quanta per  $\text{cm}^2$  and sec., i.e., by  $c$ , the density of light quanta being normalized to unity. For the emission of radiation, we had to divide by the velocity  $v_0 = cp_0/E_0$  of the primary electron; therefore we get an additional factor  $p_0 E_0/k^2 \cdot v_0/c = p_0^2/k^2$  in the cross-section (6) or (13).

There are, however, two points which have to be mentioned. Firstly, one should consider the interaction energy between the two created electrons. Fortunately, it can be seen that this interaction energy  $V_{+-}$  does not affect the calculation to our approximation. For the matrix element of  $(V_{+-})_{p_+ p_-}$  corresponding to the creation is probably the matrix element of a Coulomb interaction belonging to a transition from a positive energy state  $p_-$  to a state with negative energy and momentum  $-p_+$ , viz.,

$$(V_{+-})_{p_+ p_-} = \int d\tau \left( \exp \frac{i}{\hbar} (\mathbf{p}_- \cdot \mathbf{r}_-) \exp \left( \frac{i}{\hbar} (\mathbf{p}_+ \cdot \mathbf{r}_+) \right) \right) / |\mathbf{r}_+ - \mathbf{r}_-|. \quad (18)$$

But this matrix element vanishes except when momentum is conserved, i.e.  $\mathbf{p}_+ + \mathbf{p}_- = 0$ . It follows that, if we add to the Coulomb potential  $V$  the interaction energy  $V_{+-}$ , the latter will not contribute anything to the matrix elements occurring in (4). There will, of course, be a contribution in the next approximation which is only of the order  $e^2/\hbar v$  compared with the result of our approximation, while the application of Born's approximation means an error of the order  $Ze^2/\hbar v$ .

The second point is, that in (13) the momentum and the energy  $E$  are the momentum and energy of the hole in the "sea of negative energy electrons" which corresponds to the positive electron. The momentum and energy of the positive electron itself are  $-p$  and  $-E$ . It is, therefore, physically more significant to introduce

$$E_+ = -E, \quad \mathbf{p}_+ = -\mathbf{p}, \quad \theta_+ = \pi - \theta, \quad \phi_+ = \pi + \phi, \quad p_+ = p, \quad (19)$$

$\theta_+$  being the angle between the direction of motion of the positive electron and that of the incident light quantum, etc. If we introduce these quantities into (13), all terms involving the first power of  $E$  or  $p$  change sign, thus:

$$\begin{aligned} d\Phi = & - \frac{Z^2 e^4}{137 2\pi k^3} \frac{p_0 p_+}{dE_0} \frac{\sin \theta_0 d\theta_0 \sin \theta_+ d\theta_+ d\phi_+}{q^4} \left\{ \frac{p_+^2 \sin^2 \theta_+ (4E_0^2 - q^2)}{(E_+ - p_+ \cos \theta_+)^2} \right. \\ & + \frac{p_0^2 \sin^2 \theta_0 (4E_+^2 - q^2)}{(E_0 - p_0 \cos \theta_0)^2} + \frac{2p_0 p_+ \sin \theta_0 \sin \theta_+ \cos \phi_+ (4E_0 E_+ + q^2)}{(E_0 - p_0 \cos \theta_0)(E_+ - p_+ \cos \theta_+)} \\ & \left. - \frac{2k^2 (p_+^2 \sin^2 \theta_+ + p_0^2 \sin^2 \theta_0 + 2p_0 p_+ \sin \theta_0 \sin \theta_+ \cos \phi_+)}{(E_0 - p_0 \cos \theta_0)(E_+ - p_+ \cos \theta_+)} \right\}. \end{aligned} \quad (20)$$

The integration over the angles is naturally also identical with that for the radiation case. Formula (15) has, therefore, only to be multiplied by  $p_0^2/k^2$ ,  $dk$  to be replaced by  $dE_0$ , and  $E$  put equal to minus the energy of the positive electron. The cross-section for the creation of a positive electron with energy  $E_+$  and a negative one with energy  $E_0$  by a light quantum  $k = h\nu$  then becomes

$$\begin{aligned}\Phi(E_0) dE_0 = & \frac{Z^2}{137} \left( \frac{e^2}{mc^2} \right)^2 \frac{p_0 p_+}{k^3} dE_0 \left\{ -\frac{4}{3} - 2E_0 E_+ \frac{p_0^2 + p_+^2}{p_0^2 p_+^2} \right. \\ & + \mu^2 \left( \frac{\epsilon_0 E_+}{p_0^3} + \frac{\epsilon_+ E_0}{p_+^3} - \frac{\epsilon_+ \epsilon_0}{p_0 p_+} \right) + \left[ \frac{k^2}{p_0^3 p_+^3} (E_0^2 E_+^2 + p_0^2 p_+^2) - \frac{8}{3} \frac{E_0 E_+}{p_0 p_+} \right] \log \\ & \left. + \frac{\mu^2 k}{2p_0 p_+} \left[ \frac{E_0 E_+ - p_0^2 \epsilon_0}{p_0^3} + \frac{E_0 E_+ - p_+^2 \epsilon_+}{p_+^3} + \frac{2k E_0 E_+}{p_0^2 p_+^2} \right] \log \right\}, \quad (21)\end{aligned}$$

with

$$\epsilon_+ = 2 \log \frac{E_+ + p_+}{\mu}, \quad \log = \log \frac{E_0 k - p_0^2 + p_0 p_+}{E_0 k - p_0^2 - p_0 p_+} = 2 \log \frac{E_0 E_+ + p_0 p_+ + \mu^2}{\mu k}. \quad (21A)$$

This formula is, of course, symmetrical in  $E_0$  and  $E_+$ . An asymmetry would only arise in higher approximations and is small for high energies (*cf.* § 7). If all energies involved are large compared with  $mc^2$ , the formula reduces to

$$\Phi(E_0) dE_0 = \frac{Z^2}{137} \left( \frac{e^2}{mc^2} \right)^2 4 \frac{E_{0+}^2 E_+^2 + \frac{8}{3} E_0 E_+}{(h\nu)^3} dE_0 \left( \log \frac{2E_0 E_+}{h\nu mc^2} - \frac{1}{2} \right). \quad (22)$$

(21) and (22) will be discussed in § 8.

### § 3. Effect of Screening

It could be expected that the screening of the atomic potential by the outer electrons would have a considerable effect on the cross-section for the radiation phenomena considered in this paper, because it may be seen that a large part of the processes take place at big distances from the nucleus of the field-producing atom, *i.e.*, at places where the atomic field is no longer a Coulomb field.

1. *Differential Cross-section.*—The potential which the atom exerts on the electron occurs in formula (4) inside the matrix elements  $V_{AI}$  and  $V_{EI}$ . Both these matrix elements have the value (besides a factor  $(u' u_0)$  and  $(u'' u)$  respectively)

$$V_{AI} = V_{EI} = \int V \exp \frac{i}{\hbar c} (\mathbf{q} \cdot \mathbf{r}) d\tau, \quad (23)$$

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where  $q$  is the momentum transferred to the atom in the process. Now (23) can be brought into the form

$$V_{AI} = V_{EH} = \frac{4\pi\hbar^2c^2}{q^2} [Z - F(q)]^2, \quad (24)$$

where  $F$  is the well-known atomic form-factor

$$F(q) = \int \rho(r) \exp \frac{i}{\hbar c} (qr) d\tau, \quad (25)$$

$\rho(r)$  being the density of the atomic electrons at the distance  $r$  from the nucleus. Therefore, we can take account of the screening simply by writing  $(Z - F)^2$  instead of  $Z^2$  in formula (13), a change which is familiar from the theory of electron scattering.<sup>†</sup>

The atomic form-factor  $F$  depends on the distribution of the atomic electrons. We assume in our calculations that  $\rho(r)$  is the Fermi distribution, which, especially for heavy atoms, should be very accurate. We can, then, write

$$F = Z \mathcal{F}(qZ^{-\frac{1}{3}}), \quad (26)$$

where  $\mathcal{F}$  is a general atomic form-factor valid for all atoms. It is given numerically in several papers.<sup>‡</sup>

We can easily get an idea under which conditions the screening will have an appreciable effect. The atomic form-factor  $F$  becomes comparable with  $Z$ , if  $q/\hbar c$  is of the order (or smaller than) the reciprocal atomic radius. Now, the radius of the Fermi atom is approximately  $a_0 Z^{-\frac{1}{3}}$ ,  $a_0$  being the hydrogen radius. Therefore screening is effective if

$$q \ll \alpha = \frac{\hbar c}{a_0} Z^{\frac{1}{3}} = \frac{mc^2}{137} Z^{\frac{1}{3}}. \quad (27)$$

On the other hand,  $q$  takes its minimum value if the momentum of the electron is parallel to that of the emitted light quantum both before and after the radiation. Here  $q$  is equal to

$$q_{\min} = \delta = p_0 - p - k = E - p - (E_0 - p_0). \quad (28)$$

For energies  $E_0$  and  $E$  large compared with  $mc^2$  this reduces to

$$\delta = \frac{(mc^2)^2 \hbar v}{2E_0 E}. \quad (29)$$

<sup>†</sup> Cf., for instance, Mott and Massey, "Atomic Collisions," Oxford Univ. Press, 1934, p. 89.

<sup>‡</sup> For instance, Bethe, 'Ann. Physik,' vol. 5, p. 385 (1930).

This formula shows that the minimum momentum transferred to the atom decreases with increasing energy and becomes smaller than  $\alpha$ , if

$$E_0 E / h\nu > \frac{1}{2} 137 mc^2 Z^{-\frac{1}{2}}, \quad (30)$$

that is, about  $15mc^2$  for heavy atoms. (30) is the condition for the *screening to be effective*. We see from this condition that the screening will only be important for energies large compared with  $mc^2$ , and we can, therefore, assume throughout this section that  $mc^2$  is negligible in comparison with  $E_0$ ,  $E$  and  $h\nu$ . This assumption greatly simplifies the calculation.

2. *Integral Cross-section*.—The integration over the angles  $\theta_0$ ,  $\theta$ ,  $\phi$  is carried out in another paper†. The last part of this integration can only be carried out numerically, since the atomic form factor  $F$  of the Fermi atom is only known numerically. The result, i.e., the integral cross-section, can conveniently be written in the form

$$\Phi(v) dv = \frac{Z^2}{137} r_0^2 \frac{1}{E_0^2} \frac{d\nu}{v} [(E_0^2 + E^2)(\phi_1(\gamma) - \frac{1}{3} \log Z) - \frac{2}{3} E_0 E (\phi_2(\gamma) - \frac{1}{3} \log Z)], \quad (31)$$

where

$$r_0 = e^2/mc^2$$

is the electronic radius and

$$\gamma = 100 \frac{mc^2 h\nu}{E_0 E Z^{\frac{1}{2}}}, \quad (32)$$

and  $\phi_1$ ,  $\phi_2$  are two functions of  $\gamma$  which are given in fig. 1.‡

The quantity  $\gamma$  is proportional to  $\delta/\alpha$  and therefore determines the effect of screening. If  $\gamma = 0$ , we may call the *screening “complete.”* Indeed, the radiation cross-section is then determined entirely by the atomic radius, i.e., by  $\alpha$ , whereas the minimum momentum transfer  $\delta$  (and therefore the energy) has no longer any effect on the cross-section. The values of  $\phi_1$ ,  $\phi_2$  here are

$$\phi_1(0) = 4 \log 183, \quad \phi_2(0) = \phi_1(0) - \frac{2}{3}, \quad (33)$$

so that for very high energies,  $E_0 \gg 137 mc^2 Z^{-\frac{1}{2}}$ , the cross-section (31) becomes

$$\Phi(v) dv = \frac{Z^2}{137} \frac{r_0^2}{E_0^2} \frac{d\nu}{v} 4 \left[ (E_0^2 + E^2 - \frac{2}{3} E_0 E) \log (183 Z^{-\frac{1}{2}}) + \frac{E_0 E}{9} \right]. \quad (34)$$

For a given ratio  $h\nu/E_0$ , this cross-section is independent of  $E_0$ . This is not so if the energy becomes smaller ( $\gamma > 0$ ). The cross-section for a given  $h\nu/E_0$

† ‘Proc. Camb. Phil. Soc.’ in press. Referred to as C.

‡ It would have been more natural theoretically to put  $\gamma' = \delta/\alpha = 137 mc^2 h\nu/2E_0 E Z^{\frac{1}{2}}$ . The factor 100 instead of 137/2 has been chosen for convenience in using formula (31).

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then decreases, though slowly, with decreasing energy (the  $\phi$ 's decrease with increasing  $\gamma$ ). In the limiting case  $\gamma \gg 1$ , i.e., for energies small compared with  $137mc^2 Z^{-\frac{1}{2}}$  the screening ceases to have any effect, in agreement with our considerations in the preceding section. The cross-section is, then, given by formula (16). For energies that are a little higher, more accurately for values

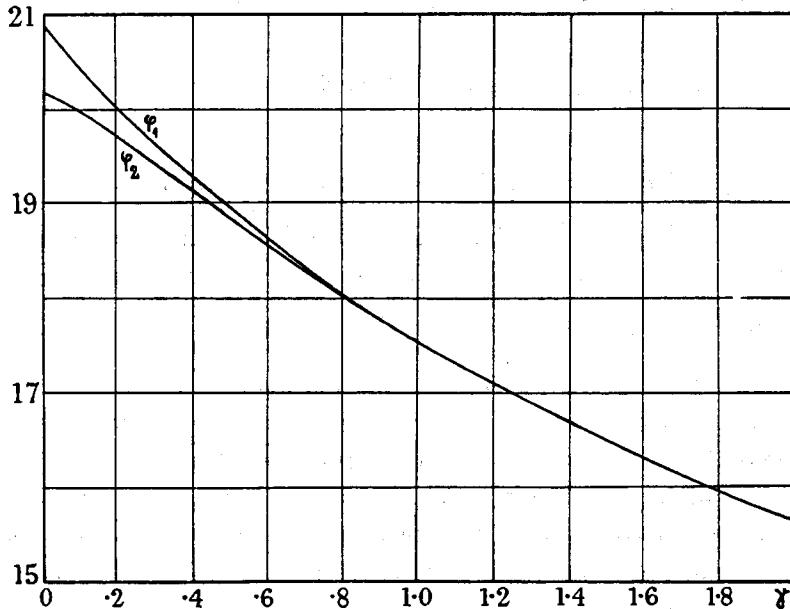


FIG. 1.— $\phi_1$  and  $\phi_2$  (cf. equation (31)) as functions of  $\gamma = 100mc^2 h\nu/E_0 E Z^{\frac{1}{2}}$ .

of  $\gamma$  between 2 and 15, the screening gives a small correction to formula (16), which may be taken into account by writing instead of (16)

$$\Phi(v) dv = \frac{Z^2}{137} \frac{r_0^2}{E_0^2} \frac{d\nu}{v} 4(E_0^2 + E^2 - \frac{2}{3}E_0 E) \left( \log \frac{2E_0 E}{mc^2 h\nu} - \frac{1}{2} - c(\gamma) \right), \quad (35)$$

and inserting for  $c(\gamma)$  the value given in Table I.

Table I.

$c(\gamma) = 0.21$	$0.16$	$0.13$	$0.09$	$0.065$	$0.05$	$0.03$	$0.02$	$0.01$	(35A)
$\gamma = 2$	$2.5$	$3$	$4$	$5$	$6$	$8$	$10$	$15$	

For the *creation of pairs* of electrons, all formulæ are exactly similar except for the normalizing factor and for the sign of  $E$ . If, in accordance with § 2, we call the energy of the positive electron  $E_+$ , the cross-section for creation becomes

$$\Phi(E_0) dE_0 = \frac{Z^2}{137} r_0^2 \frac{dE_0}{(h\nu)^3} [(E_0^2 + E_+^2)(\phi_1(\gamma) - \frac{4}{3} \log Z) + \frac{2}{3}E_0 E_+(\phi_2(\gamma) - \frac{2}{3} \log Z)], \quad (36)$$

$\phi_1(\gamma)$  and  $\phi_2(\gamma)$  being the functions shown in fig. 1, and

$$\gamma = 100mc^2 h\nu Z^{-\frac{1}{2}} / E_0 E_+.$$

For small energies the formula

$$\Phi(E_0) dE_0 = \frac{Z^2}{137} r_0^2 \frac{dE_0}{(h\nu)^2} (E_0^2 + E_+^2 + \frac{2}{3} E_0 E_+) 4 \left( \log \frac{2E_0 E_+}{h\nu mc^2} - \frac{1}{2} - c(\gamma) \right), \quad (37)$$

is more convenient,  $c(\gamma)$  being given in Table I (35A).

#### § 4. Radiation Probability as Function of Impact Parameter

It is possible to get a rough idea about the probability that an electron passing at a given distance  $r$  from the nucleus emits radiation during its passage. For the main contribution to the matrix element  $V(q) = \int V \exp i(\mathbf{qr})/\hbar c \cdot d\tau$  arises from the region  $r \sim \hbar c/q$ , since the contribution of larger  $r$ 's nearly vanishes because of interference, while small  $r$ 's do not contribute appreciably, because of the smallness of the corresponding volume. Therefore, the radiation emitted in the region between  $r$  and  $r + dr$  will be equal to the probability of a radiation process in which a momentum between  $q = \hbar c/r$  and  $q + dq$  is transferred to the atom. This probability  $\Phi(q) dq$  has been calculated in the paper (C) referred to above (§ 7), viz.,

$$\Phi(q) dq \sim (1 - \mathcal{F}(q))^2 dq/q \quad \text{if } q \ll \mu, \quad (38)$$

$$\Phi(q) dq \sim (\log(q/\mu) + \text{const.}) \cdot dq/q^3 \quad \text{if } q \gg \mu. \quad (39)$$

(cf. C. (67), (66)) since the number of incident electrons having a minimum distance from the nucleus (impact parameter) between  $r$  and  $r + dr$  is proportional to  $r dr$ , we get for the probability that an electron passing at a distance  $r$  radiates

$$\Phi(r) = \Phi(q) \frac{dq}{r dr} \sim \Phi(q) r^{-3}. \quad (40)$$

If  $r$  is smaller than the Compton wave-length  $\hbar/mc$ ,  $q$  will be larger than  $mc^2$ . For this case we take from (39)

$$\Phi(r) = \text{const.} \log \frac{\hbar}{mc} r \quad (\text{for } r \ll \hbar/mc). \quad (39A)$$

That means that for small  $r$  the radiation emitted at distances between  $r$  and  $r + dr$  is nearly independent of  $r$ . On the other hand, for  $r$  larger than  $\hbar/mc$ ,

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$q$  will be small compared with  $\mu$ . If  $q$  is still large compared with  $\alpha$ , then, according to (27),  $\mathcal{F}(q)$  may be neglected in (38). Thus,

$$\Phi(r) \sim 1/r^2 \quad (\text{if } \hbar/mc \ll r \ll a_0 Z^{-\frac{1}{3}} \text{ and } r \ll \hbar/mc \cdot E_0 E / h v m c^2). \quad (38A)$$

The second condition follows from (29). If  $r$  increases, (38A) will cease to hold. The point at which this occurs depends on whether the energy  $E_0$  is larger or smaller than  $137mc^2 Z^{-\frac{1}{3}}$ . In the first case, this limit  $r_{\max}$  is given by the atomic radius. Then, for distances larger than  $r_{\max} = a_0 Z^{-\frac{1}{3}}$  screening becomes appreciable and causes  $\Phi(q)$  to decrease like  $q^3$ , (cf. C (69) which means

$$\Phi(r) \sim 1/r^6 \quad (\text{for } r \gg a_0 Z^{-\frac{1}{3}}). \quad (41)$$

If, on the other hand, the energy is small compared with  $137mc^2 Z^{-\frac{1}{3}}$ , formula (38A) ceases to be valid already at the point  $r_{\max} = \hbar/mc \cdot E_0 E / h v m c^2$  (corresponding to  $q$  of the order  $\delta$ ).

The main contribution to the total cross-section is given by the region (38A) because the region of smaller  $r$ 's (39A) has only a small volume, and for large  $r$ 's the radiation probability falls off very rapidly. Therefore the total cross-section will be proportional to

$$\int_{\hbar/mc}^{r_{\max}} \Phi(r) r dr = \log \frac{r_{\max}}{\hbar/mc} = \begin{cases} \log \frac{a_0 Z^{-\frac{1}{3}}}{\hbar/mc} & \text{for } E_0 > 137mc^2 Z^{-\frac{1}{3}} \\ \log \frac{E_0 E}{h v m c^2} & \text{for } E_0 < 137mc^2 Z^{-\frac{1}{3}} \end{cases}, \quad (42)$$

which agrees roughly with the results (16), (34) of our exact calculations.

The absolute radiation probability for an electron passing the nucleus at a distance smaller than  $\hbar/mc$  is of the order†  $Z^2/137^3$ , which is very small, even for the heaviest atoms. This behaviour is very different from the result of classical electrodynamics, according to which the total energy radiated should increase as  $r^{-3}$  (cf. paper I § 6) if the electron passes near the nucleus, and should become equal to the primary energy of the electron for  $r = r_0 Z^{\frac{1}{3}} \left(\frac{E_0}{mc^2}\right)^{\frac{1}{3}}$ .

It would seem from this comparison that the quantum mechanical treatment yields a much smaller radiation probability; but nevertheless even this seems to be too large compared with the experiments (cf. § 7‡).

† These electrons form a beam of diameter  $2\hbar/mc$ . To obtain the radiation probability for a single electron, we have to divide the radiative cross-section for these electrons which is certainly smaller than the total cross-section, i.e.,  $\sim r_0^2 Z^2/137$ , by the area  $\pi(\hbar/mc)^2 = \pi \cdot (137 r_0)^2$ .

‡ Similar results to those mentioned in this section have been derived by a semi-classical consideration by Weizsäcker, to whom we are indebted for the communication of his results.

## II. DISCUSSION

§ 5. *The Radiation Emitted by Fast Electrons*

1. *Intensity Distribution.*—In § 1 and 3, we have calculated the probability that an electron of energy  $E_0$  emits a light quantum of frequency between  $\nu$  and  $\nu + d\nu$  (equations (15) and (31)). This probability is roughly proportional to  $1/\nu$  and consequently becomes very large for the emission of quanta of low

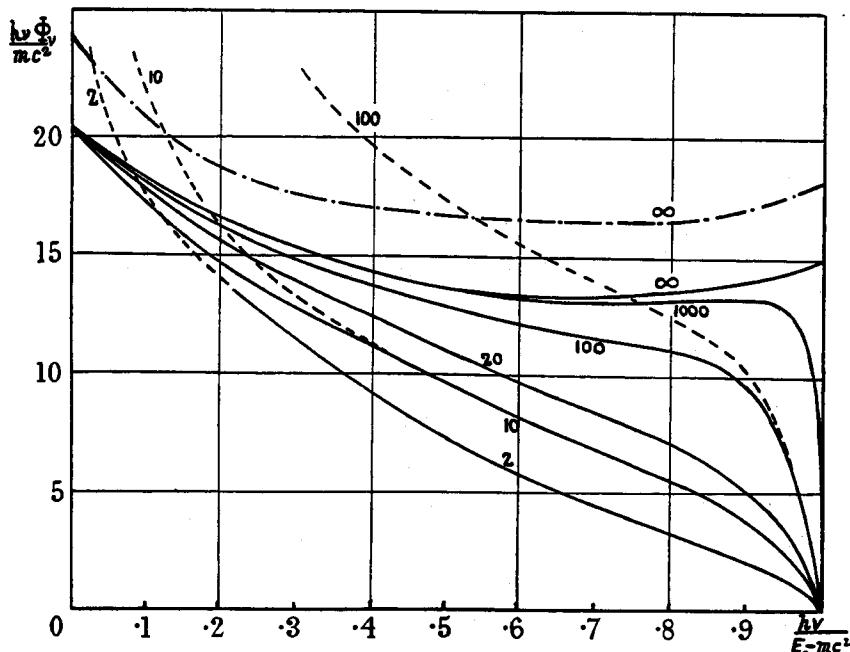


FIG. 2.—Intensity distribution  $h\nu\Phi_0$  of the emitted radiation for Pb (—),  $H_2O$  (---), and with screening neglected (- - -).  $\Phi_0$  is the cross-section in units  $Z^2\tau_0^2/137$ . The numbers affixed to the curves refer to the primary energy  $E_0$  in units  $mc^2$ .

energy. We have, therefore, plotted in fig. 2 the *intensity* of the emitted radiation, *i.e.*, frequency times the probability of emission, rather than the probability itself as function of the frequency. Fig. 2 shows the intensity distribution for Pb,  $H_2O$  and for the case where the screening is neglected.†

† The general behaviour of the intensity frequency curves is similar to that which follows for the radiation of slow electrons ( $\nu \ll c$ ) from the *exact* but non-relativistic Sommerfeld theory ('Ann. Physik,' vol. 11, p. 302 (1931), fig. 7). The two theories differ, however, for very small and very high frequencies : for  $\nu = 0$  the intensity becomes logarithmically infinite in Sommerfeld's theory, finite in ours. This is due to the neglection of screening in Sommerfeld's calculation ; in our theory the same infinity appears if we

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The cross-section  $\Phi$ , is expressed in units  $Z^2 r_0^2 / 137$  in order to make its values for different atoms comparable.

The intensity decreases with increasing frequency, and falls to zero at the short wave-length limit  $(E_0 - mc^2)/h$ .

The intensity of the soft radiation, even in units  $Z^2$ , is dependent on the atomic number  $Z$  (increasing for small  $Z$ ), but independent of the energy  $E_0$  of the incident electron.

The intensity of the harder radiation ( $v \sim v_0$ ) increases slowly with increasing energy (if  $v/v_0$  is kept constant) and reaches a certain asymptotic value for high  $E_0$ , which depends on the atomic number  $Z$ .

2. *The number of emitted quanta* in a given frequency interval  $v$  to  $v + dv$  is

$$n(v) = dv \int_{hv}^{E_i} \frac{N \Phi(v, E_0) dE_0}{-dE_0/dx}, \quad (43)$$

where  $E_i$  is the initial energy of the emitting electron,  $-dE_0/dx$  is its energy loss per centimetre path,  $\Phi(v, E_0)$  the cross-section for the emission of a quantum of frequency  $v$  by an electron of energy  $E_0$  as given by formulæ (15), (31), and  $N$  the number of atoms per unit volume. To a rough approximation,  $hv \Phi(v, E_0) = K$  may be considered as independent of  $v$  and  $E_0$ , fig. 2. The energy loss of the electron is for large energies  $E_0$  mainly due to radiation, as is proved in § 6, if this is so,  $-dE_0/dx = KE_0$ . This formula holds down to a critical energy  $E_c = 1600mc^2/Z$  (equation (52)), below which the energy loss due to collisions becomes important. This latter is, then, much greater than  $E_0K$  so that the contribution of  $E < E_c$  to (43) may be neglected. Therefore, roughly, we have

$$\left. \begin{aligned} n(v) &= \frac{dv}{v} \log \frac{E_i}{E_c} && \text{for } hv < E_c < E_i \\ n(v) &= \frac{dv}{v} \log \frac{E_i}{hv} && \text{for } E_c < hv < E_i \end{aligned} \right\}. \quad (44)$$

use the non-screened formula (15) as we see from the dotted curves in fig. 2. On the other hand, at the short wave-length limit our theory is, presumably, not correct. For, we have made use of Born's first approximation which goes wrong if the energy of the electron after the radiation is small (cf. § 1). The exact wave-functions are, in this case, much larger near the nucleus than Born's wave-functions of first approximation. Consequently, the transition probability becomes also much larger, and the intensity of the radiation at any rate does not drop so much as shown in fig. 2. It seems plausible that actually it would tend to a finite limit for  $v \rightarrow v_0$ , as it does in Sommerfeld's exact theory.

If an electron of initial energy  $E_i = 137mc^2$  (limit of validity of our theory, cf. § 7) is stopped in lead ( $E_e = 20mc^2$ ) there will in the average be emitted :—

quanta of energy	>50	20-50	10-20	5-10	2-5	1-2 $mc^2$
number .....	0.5	1.5	1.5	1.5	2	1.5

altogether 8.5 quanta of energy greater than  $mc^2$ .

This table has been calculated from the crude formula (44), since we wanted only to show the order of magnitude ; actually there are fewer large quanta and rather more small quanta, owing to the intensity distribution in the spectrum (fig. 2).

3. *Angular Distribution of Emitted Radiation.*—The radiation of fast electrons ( $E_0 \gg mc^2$ ) is emitted mainly in the forward direction. The average angle between the directions of motion of the electron and the emitted light is of the order  $\Theta = mc^2/E_0$  (cf. paper C, § 8).

#### § 6. Energy Loss of Fast Electrons by Radiation.

1. *Calculation of Energy Loss.*—The average energy radiated by an electron of energy  $E_0$  per centimetre of its path is

$$-\left(\frac{dE_0}{dx}\right)_{\text{rad}} = N \int_0^\infty h\nu \Phi d\nu, \quad (45)$$

$N$  being the number of atoms per  $\text{cm}^3$  and  $\Phi$ , the cross-section given by equations (15), (31). The integration over  $\nu$  can, in general, only be carried out numerically. There are, however, two cases in which analytical integration is possible : (1) if  $E_0$  is so small that screening has no effect at all

$$E_0 \ll 137mc^2Z^{-\frac{1}{3}},$$

and yet  $E_0$  is large compared with  $mc^2$ ; (2) if the energy  $E_0$  is so high that the asymptotic formula (34) is valid for all values of  $\nu$  (complete screening  $E_0 \gg 137mc^2Z^{-\frac{1}{3}}$ ). In the first case, formula (16) may be used for  $\Phi$ . The integration yields

$$-\left(\frac{dE_0}{dx}\right)_{\text{rad}} = N \frac{Z^2}{137} r_0^2 E_0 \left( 4 \log \frac{2E_0}{mc^2} - \frac{4}{3} \right) \quad (\text{for } mc^2 \ll E_0 \ll 137mc^2Z^{-\frac{1}{3}}). \quad (46)$$

This formula has already been published in a preliminary note by Heitler and Sauter.<sup>†</sup> It differs from the estimation (1) given in I by the logarithmic term, which varies only very slowly with the primary energy  $E_0$ .

<sup>†</sup> 'Nature,' vol. 132, p. 892 (1933).

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For very high energies (case 2) the integration gives

$$-\left(\frac{dE_0}{dx}\right)_{\text{rad}} = N \frac{Z^2 r_0^2}{137} E_0 \left(4 \log 183 Z^{-\frac{1}{2}} + \frac{2}{9}\right) \quad (\text{for } E_0 \gg 137mc^2 Z^{-\frac{1}{2}}), \quad (47)$$

which means a cross-section independent of  $E_0$ .

The result of the numerical integration in the intermediate range and for small energies is shown in fig. 3. For convenience of representation, we have plotted the "integrated cross-section  $\Phi_{\text{rad}}$  in units  $Z^2 r_0^2 / 137$ ," defined by

$$-\left(dE_0/dx\right)_{\text{rad}} = NE_0 Z^2 r_0^2 / 137 \cdot \Phi_{\text{rad}}, \quad (48)$$

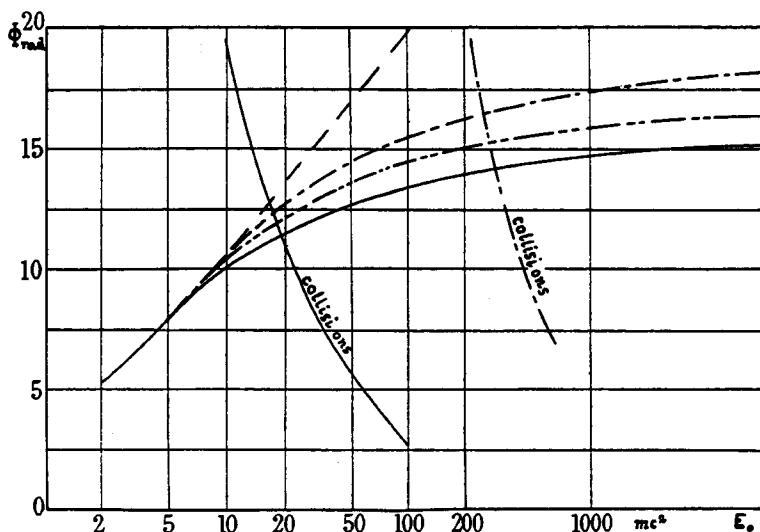


FIG. 3.—Cross-section  $\Phi_{\text{rad}}$  for the energy loss by radiation (defined in equ. 48) as a function of the primary energy for Pb (—), Cu (---), H<sub>2</sub>O (— · —) and with screening neglected (— · — · —). For comparison the cross-section for the energy loss by collisions for Pb and H<sub>2</sub>O are shown on the same scale.

against  $\log_{10} E_0$  for three values of  $Z$ .  $\Phi_{\text{rad}}$  increases but slowly with increasing energy and decreasing atomic number. For comparison, we have plotted the cross-section for *energy-loss by collisions* in the same units  $Z^2 r_0^2 / 137$ .

$\Phi_{\text{rad}}$  being a slowly varying function, the radiative energy loss is approximately proportional to the initial energy of the electron  $E_0$ , whereas the energy loss by collisions is approximately constant. Further, the energy loss by radiation is proportional to  $Z^2$ , whereas the energy loss by collisions is proportional to  $Z$ . No universal mass absorption-coefficient exists, therefore, for the radiative energy loss.

Table II.—Energy Loss of Fast Electrons by Radiation and Collisions  
in millions of volts per centimetre path.

Substance.	Energy loss.	Energy of electron in million volts.						
		5	10	20	50	100	300	1000
$H_2O$	Radiation	0.07	0.16	0.36	0.99	2.07	6.6	22.5
	Collisions	1.98	2.15	2.32	2.55	2.72	2.99	3.29
Cu	Radiation	2.1	4.9	10.9	28.9	61	191	660
	Collisions	12.7	14.0	15.2	0.7	18.2	20.3	22.5
Pb	Radiation	6.4	14.4	31.4	85	177	550	1900
	Collisions	12.5	13.9	15.3	17.3	18.6	20.9	23.4

Table II gives the absolute value of the energy loss for various substances.

The energy loss by radiation is seen to be much greater, for high energies  $E_0$ , than the ordinary energy loss by inelastic collisions. The latter has been calculated from the usual formula for electrons with relativistic energy  $> mc^2$ , namely,

$$-\left(\frac{dE_0}{dx}\right)_{\text{coll}} = 2\pi r_0^2 mc^2 Z N \log \frac{E_0^3}{2mc^2 I^2}. \quad (49)$$

Following the theory of Bloch (*loc. cit.*), the average ionization potential  $I$  was assumed to be proportional to the atomic number  $Z$ , explicitly

$$I = 13.5 \cdot Z \text{ volts}, \quad (50)$$

the proportionality factor 13.5 being redetermined for this purpose from the observed energy loss of fast  $\alpha$ -particles in gold.<sup>†</sup>

The ratio of radiation and collision energy loss is roughly

$$\frac{-(dE_0/dx)_{\text{coll}}}{-(dE_0/dx)_{\text{rad}}} = \frac{E_0 Z}{1600 mc^2}. \quad (51)$$

This simple formula is due to the fact that the logarithm in (49) varies with  $E_0$  and  $Z$  in approximately the same way as that in (48). Radiation and collision become of equal importance at the "critical" energy

$$E_c = 1600 mc^2/Z, \quad (52)$$

i.e., about  $20 mc^2 = 10$  million volts for lead,  $55 mc^2$  for copper,  $200 mc^2$  for air.

<sup>†</sup> No account was taken of the excitation of nuclear electrons, since it seems highly improbable that the probability of this excitation (if it occurs at all) can be calculated by the simple wave-mechanical formula (49), considering that the electrons presumably do not exist at all in the nucleus. We think that the excitation of nuclear electrons rarely takes place.

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2. The range of the electron is determined by the quantity

$$-\left(\frac{dE_0}{dx}\right)_{\text{rad}} - \left(\frac{dE_0}{dx}\right)_{\text{coll}}.$$

For a rough estimate we may consider  $\Phi_{\text{rad}}$  in (48) as a constant and insert for it an average value  $\Phi_0$ , say. Then, according to (48), (51), (52), the whole energy loss is given by

$$-\frac{dE_0}{dx} = N \frac{Z^2}{137} r_0^2 \Phi_0 (E_0 + E_c), \quad (53)$$

the first term ( $E_0$ ) representing the radiation ( $E_0$  being the energy after  $x$  cm. path), the second ( $E_c$ ) the collisions ( $E_c$  being constant). Integrating (53) we get for the range the rough formula

$$R = \frac{137}{NZ^2 r_0^2 \Phi_0} \log \frac{E_0 + E_c}{E_c} = \frac{137}{NZ^2 r_0^2 \Phi_0} \log \left(1 + \frac{ZE_0}{1600mc^2}\right). \quad (54)$$

The range of high energy electrons increases, according to (54), only with the logarithm of the energy and remains, therefore, very small even for the fastest electrons. Table III gives the result of an exact numerical calculation of the range in Pb, Cu, H<sub>2</sub>O; for Pb the range calculated by the rough formula (54) is added to show the accuracy of this formula.

Table III.—Average Range of Fast Electrons in cm.

Stopping material.	Energy in million voltae.							
	5	10	20	50	100	300	1000	10000
H <sub>2</sub> O .....	2.5	4.8	8.8	18.4	30.4	58	100	195
Cu .....	0.37	0.67	1.12	1.96	2.78	4.25	6.0	9.4
Pb .....	0.33	0.54	0.81	1.23	1.68	2.25	2.88	4.08
Pb (calculated by (54)) .....	0.25	0.43	0.68	1.12	1.50	2.14	2.87	4.30

3. *Straggling*.—The effect of radiation is to diminish the energy of an electron suddenly by rather a large fraction of its initial value. Therefore, the actual energy loss may differ very considerably from the average loss. To obtain a rough idea of the effect of this straggling, we assume for the probability of emission of a light quantum  $h\nu$  a rough but convenient formula :

$$\Phi(\nu) d\nu = a \frac{d\nu}{E_0 \log E_0/E}, \quad (55)$$

where  $a$  is a constant.

(55) may be seen to represent the intensity curves  $h\nu \Phi$ , of fig. 2 fairly well. If we introduce instead of  $\nu$

$$y = \log [E_0/(E_0 - h\nu)] \quad (56)$$

(which is convenient since on the average the log of the electronic energy decreases linearly with the distance), the probability that the electron loses the energy  $\hbar\nu$  in travelling an *infinitely short distance*  $dl$  is

$$w(y) dy = \Phi(\nu) d\nu dl = a \frac{e^{-\nu}}{\nu} \frac{dy}{y} dl. \quad (57)$$

We wish to know the probability for a decrease of the energy of the electron to  $e^{-y}$  times its initial value after traversing matter of a *finite thickness*  $l$ . For this probability we can prove the following formula to be correct :

$$w(y) dy = \frac{e^{-y} y^{al-1}}{\Gamma(al)} dy \quad (58)$$

(58) becomes identical with (57) for very small  $l$ . For, in this case

$$\Gamma(al) = 1/al \quad \text{and} \quad y^{al} = 1$$

(except for the smallest values of  $y$ , i.e., for the smallest values of  $\nu$ ).

To prove that (58) holds for finite  $l$ , we let the electron travel first a distance  $l_1$  then a distance  $l_2$ . The log of the energy decreases first by  $y_1$ , then by  $y_2$  altogether by  $y = y_1 + y_2$ . If (58) is assumed to be correct for the two parts of the path, the probability of the decrease  $y$  becomes :

$$w(y) dy = dy \int_0^y w_1(y_1) w_2(y-y_1) dy_1 = dy \frac{e^{-y}}{\Gamma(al_1) \Gamma(al_2)} \int_0^y y_1^{al_1-1} (y-y_1)^{al_2-1} dy_1. \quad (59)$$

The integral is evidently proportional to  $y^{a(l_1+l_2)-1}$ . The numerical factor follows from the fact that  $\int_0^\infty w(y) dy = 1$ . Therefore, if (58) is valid for the energy losses in the paths  $l_1$  and  $l_2$ , it is also valid for the energy loss in the total path  $l = l_1 + l_2$  and is thus proved to hold for any length of the path.

The curves in fig. 4 give the probability that an electron which loses energy only through radiation has, after travelling a certain distance  $l$ , still an energy left which is greater than  $e^{-1}, e^{-2}, \dots$ , times its initial energy. The abscissa is  $al$ . Now the *average energy loss*  $\bar{y}$  is exactly equal to  $al$ , if the law (57) is accepted. (This can easily be seen by calculating  $\int y w(y) dy$  from (58).)

For instance, in the *average* the energy is diminished to  $e^{-1}$  times its initial value after travelling a distance  $al = 1$ , but, as can be seen from fig. 4, even after so great a distance as  $la = 2.8$  there still remains a probability of 10% that the energy is higher than  $e^{-1} E_0$ . Thus the straggling may increase the

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range of some electrons to twice or even three times its average value ; on the other hand, some electrons are stopped much earlier.

The straggling is characteristic of the energy loss by radiation. By this effect, the latter differs from the energy loss by collisions. The unambiguity of this distinction may be seen from Table IV, in which the distribution of energy losses is given for an electron of 50 million volts primary energy traversing  $\frac{1}{2}$  mm. of lead, assuming (a) that only collisions take place, (b) only radiation, (c) both. The last two lines give the distribution after traversing 1 mm. lead for initial energies of 50 and 10 million volts.

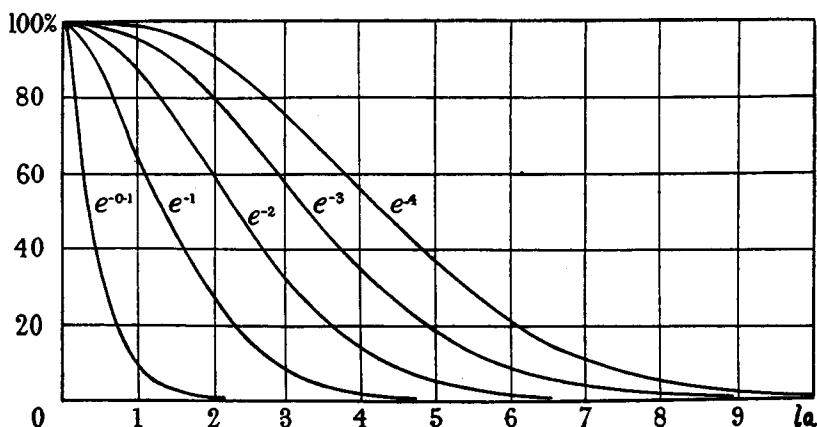


FIG. 4.—Straggling. Probability that an electron after having travelled  $l$  cm. has still an energy greater than  $e^{-1}$ ,  $e^{-2}$ , ..., times its initial energy. The scale of the abscissa is chosen so that in the average the energy decreases to  $e^{-l\alpha}$ .

Table IV.—Probability of different Energy Losses for Electrons passing through Lead (%).

Initial energy.	Thickness of Pb.	Energy lost by	Energy loss in million volts.									
			<0.1	0.1-0.5	0.5-0.7	0.7-1	1-2	2-3	3-5	5-10	10-20	20-50
50	$\frac{1}{2}$ mm.	Collision	0	0	58	32	7.5	1	0.7	0.4	0.2	0.2
50	$\frac{1}{2}$ mm.	Radiation	49	12.4	2.7	2.8	5.9	3.6	4.5	6.2	5.9	6.7
50	$\frac{1}{2}$ mm.	Both	0	0	29	25	14	5.0	7.3	7.0	6.1	6.6
50	1 mm.	Both	0	0	0	0	35	12	11	14	12	16
10	1 mm.	Both	0	0	0	0	57	16	13	14	—	—

### *§ 7. Comparison with Experiment. Limits of the Quantum Theory.*

1. *The theoretical energy loss by radiation for high initial energy is far too large to be in any way reconcilable with the experiments of Anderson.*† He has measured the energy loss of electrons of initial energy  $300 \cdot 10^6$  volts and found

† Anderson, 'Phys. Rev.', vol. 44, p. 406 (1933).

it to be about  $35 \cdot 10^6$  volts per cm. of lead as against  $550 \cdot 10^6$  volts given in our theoretical table. The disagreement is definite, although there are several reasons why a more exact theory may give a lower value for the energy loss.

(1) The figures given in Table II apply to electrons having really the energy  $E_0$ . Actually, when the electron has travelled a certain distance, say, 1 mm., it has lost some energy, and therefore the energy loss in the second millimetre will be less than in the first. Thus, the actual range of the electrons will not be  $300/550 = 0.55$  cm., but about 2 cm. (cf. Table III). Even so, the electron should lose in 1 cm. of lead about 250 million volts, i.e., nearly all its energy.

(2) It is not quite correct to base the arguments on the average loss of energy, because in each radiation process rather a large fraction of the energy is lost. Therefore, the actual energy loss may for some electrons be considerably smaller than the average (straggling, § 6, section 3). But, since Anderson has measured rather a large number of electron tracks, it seems inconceivable that all his electrons should have lost particularly small amounts of energy.

(3) Our calculations are based on Born's method which may be wrong for such heavy atoms as lead (§ 1). The error, however, should not be appreciable, since the creation of positive electrons seems to be in good accord with our calculation for energies  $2-10 mc^2$  (§ 8); in particular the creation probability is found experimentally to be very nearly proportional to  $Z^2$  as required by Born's approximation. Since the calculations for creation of pairs and for emission of radiation are absolutely analogous, it is impossible that Born's approximation can be far wrong for the radiation case. Therefore, even allowing for the three corrections, it seems impossible that the theoretical energy loss can be smaller than about 150 million volts per centimetre lead for Anderson's electrons. The theory gives, therefore, quite definitely a wrong result.†

This can perhaps be understood for electrons of so high an energy. The de Broglie wave-length of an electron having an energy greater than  $137 mc^2$  is smaller than the classical radius of the electron,  $r_0 = c^2/mc^2$ . One should not expect that ordinary quantum mechanics which treats the electron as a point-charge could hold under these conditions. It is very interesting that the energy loss of fast electrons really proves this view and thus provides *the first instance*

† We do not think that the fact that the cosmic radiation reaches the bottom of Lake Constance is equally conclusive. For the highly penetrating radiation may consist of heavy particles; for instance, protons. For these the radiation probability would be almost zero, being inversely proportional to the square of the mass.

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*in which quantum mechanics apparently break down for a phenomenon outside the nucleus.* We believe that the radiation of fast electrons will be one of the most direct tests for any quantum-electrodynamics to be constructed.<sup>†</sup>

2. It appears, therefore, to be of great importance indeed to test the radiation formulæ for energies for which they should be valid, i.e.,  $E_0 < 137 mc^2$ . Even here there is a region where the *energy loss by radiation is much bigger than the energy loss by collisions*. For lead, this region lies between 10 and  $50 \times 10^6$  volts. The only electrons at present available in the required energy range seem to be those in the showers of cosmic radiation. Unfortunately they always occur associated with so many other electrons that it should be rather difficult to test directly the emission of radiation by such electrons.

Therefore, the only means of detecting the radiation is the straggling of the energy loss of the shower electrons. To decide unambiguously whether this energy loss is due to ordinary inelastic collisions or to radiation, it would be best to investigate the loss in rather thin metal plates, say, 1 mm. thick. Then most of the electrons will undergo only collisions and will, thus, lose about 1.5 or 2 million volts while a few will lose a considerable fraction of their initial energy (cf. § 6, Table III).

Another test for the energy loss by radiation would be its dependence on the nuclear charge  $Z^2$ . The energy loss per gm./cm.<sup>2</sup> in Pb would, for electrons of an energy between 10 and 50 million volts, be much bigger than in Al, whereas it would be almost the same if the energy loss were due to collisions only.

The theory could, perhaps, also be proved in the region of fast  $\beta$ -particles for which the radiation probability is already very large. If one chooses a suitable substance which emits no  $\gamma$ -rays, the radiation emitted by the  $\beta$ -particles could be measured directly. Or one could investigate the Wilson tracks in a heavy gas such as xenon or a compound containing lead and detect directly the points where energy is lost without production of a branch track. In xenon the probability that the electron loses more than 1/10 of its energy in a radiation process is about 1 : 1000 per centimetre (electron energy  $2-10 mc^2$ ).

<sup>†</sup> A very interesting attempt has recently been made by Born to change the classical field equations so as to take the electron radius into account. He found that, for wavelengths  $\lambda < r_e$ , one has to replace the electronic charge  $e$  by an "effective charge" which decreases rapidly with decreasing  $\lambda/r_e$ . This would, of course, immediately decrease the radiative energy loss. Cf., 'Nature,' vol. 132, pp. 282, 970, 1004 (1933); vol. 133, p. 63 (1934); and 'Proc. Roy. Soc.,' A, vol. 143, p. 410 (1934). An exact comparison with experiments is not yet possible, since up to the present the quantum translation of Born's theory has not been developed sufficiently.

Finally, the stopping in a thin solid plate would give a more conclusive result than for shower-electrons, because many more particles are available. But the experiments with  $\beta$ -particles would, of course, not make experiments on shower-electrons unnecessary, because one wants to see at what energy the quantum theory *begins* to give wrong results.

3. The lowest cosmic ray electron for which the energy loss has been measured was one of 113 million volts. This is still outside the region where quantum mechanics is expected to apply, but not very much above the limit of  $137 mc^2$ . Anderson found the energy loss in a lead plate of 13.5 mm. thickness to be about  $27 \cdot 10^6$  volts, i.e.,  $20 \cdot 10^6$  volts per centimetre. This is only slightly more than would be expected for collisions only. If other tracks of this energy should give similar results, one would, therefore, conclude that already for this energy the quantum theory gives far too high a radiation probability. But it may be that this particular electron has, by chance, not emitted any large quantum. The question of the validity of our formulæ for the radiation of electrons with energy smaller than  $137 mc^2$  can thus only be decided when further experiments are available.

On the other hand, the measured energy loss of  $35 \cdot 10^6$  volts for the 300 million volt electron seems to indicate that not only inelastic collisions are effective in the stopping of fast electrons.<sup>†</sup> We should like to attribute the difference to emission of radiation.

### § 8. Creation of Positive Electrons.

1. *Energy Distribution.*—The probability that a  $\gamma$ -ray-quantum of energy  $h\nu$  creates a positive electron with energy between  $E_+$  and  $E_+ - dE_+$ , and a negative one with energy between  $E_0$  and  $E_0 + dE_0$ , is given by—

Formula (21), if  $h\nu$  is of the order  $mc^2$ ;

Formula (22), if  $h\nu \gg mc^2$ , but  $h\nu \ll 137 mc^2/Z^4$ ;

Formula (36), if  $E_0 E_+ / h\nu mc^2$  is of the order  $137 mc^2/2Z^4$  or larger.

The results of these formulæ are shown in figs. 5 (a) and 5 (b). The quantity actually plotted is the cross-section  $\Phi_{E_+}$  in units  $r_0^2 Z^2/137$ .

The abscissæ denote  $(E_+ - mc^2)/(h\nu - 2mc^2)$ , i.e., the kinetic energy of the positive electron as a fraction of the sum of the kinetic energies of both electrons.

<sup>†</sup> It should be expected that the exact quantum electrodynamics would give rather a lower energy loss in collisions than the quantum theory which itself gives only  $20 \cdot 10^6$ .

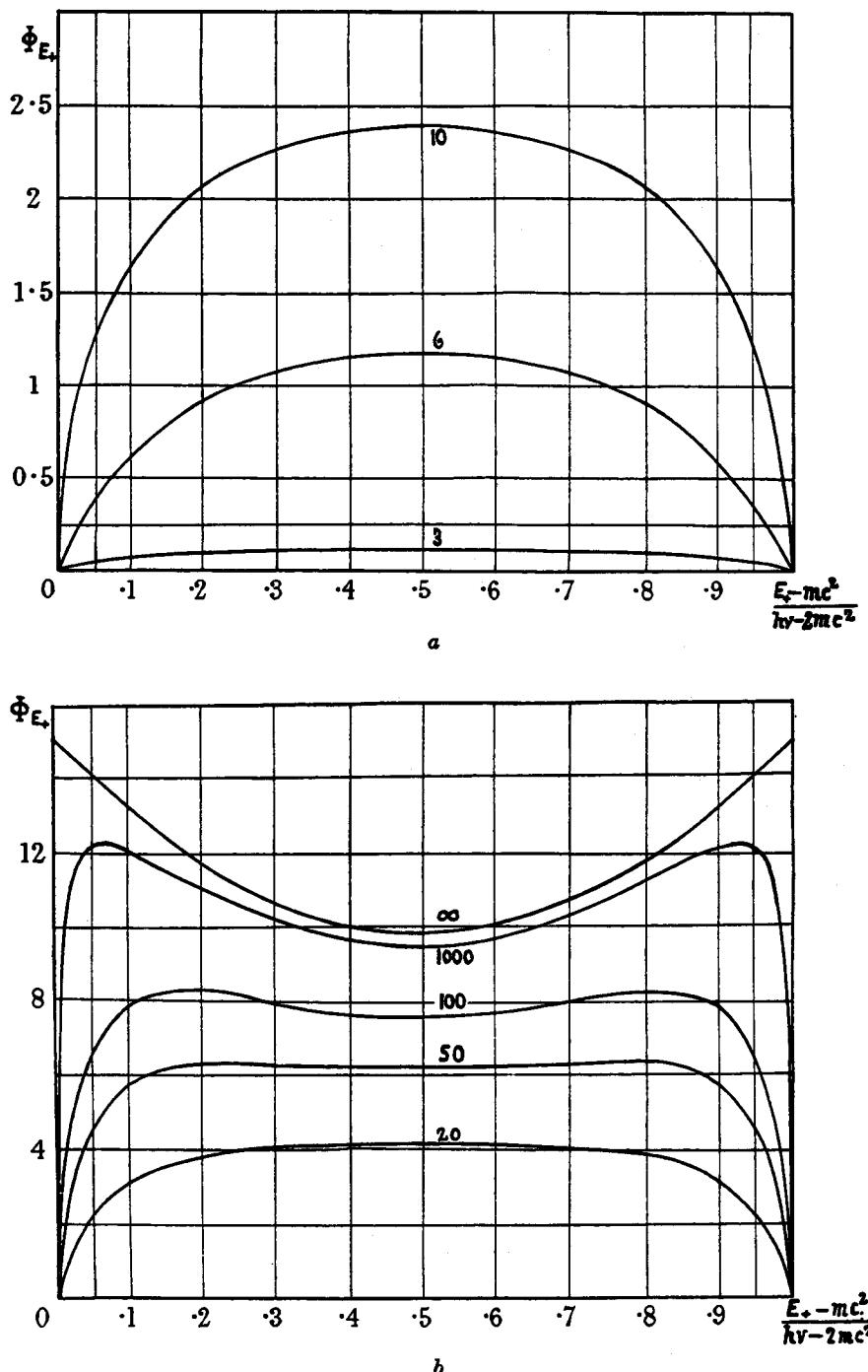
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FIG. 5.—Energy distribution of pairs of positive and negative electrons.  $\Phi_{E+}$  is the cross-section (units  $Z^2 r_0^2 / 137$ ) for the creation of a positive electron with kinetic energy  $E_+ - mc^2$ . The numbers affixed to the curves refer to the energy of the light quantum  $h\nu$  in units  $mc^2$ . Fig. 5a is valid for any element (screening neglected), fig. 5b refers to lead.

The curves for small values of  $h\nu$  are valid for any element, those for  $h\nu > 50mc^2$  are calculated for lead, for lighter elements  $\Phi_{E+}$  would be a little larger because of the smaller effect of screening, but the general form of the curves would be the same.

For quanta of small energy the probability of creation has a broad maximum when both electrons obtain equal energy. The maximum becomes flatter with increasing energy. For higher energies the probability has a flat minimum for equal energy and a small maximum when one of the electrons obtains much more energy than the other. This change of the form of the curves can be seen directly from the formulæ (22) and (36).†

The energy distribution is apparently symmetrical in the energies of the two electrons. This is a consequence of the use of Born's approximation. In an exact calculation, the positive electron would be found to obtain more energy, on the average, than the negative, as has been pointed out by several authors. This is due to the repulsion of the positive electron and the attraction of the negative by the nucleus. If the electrons are generated at a distance  $r$  from the nucleus, the energy difference of the two electrons will be  $2Ze^2/r$ .

Now according to § 4 the main contribution to the cross-section arises from a region between  $\hbar/mc$  and  $(\hbar/mc)(h\nu/2mc^2)$  provided that  $h\nu \ll 137 mc^2 Z^{-\frac{1}{3}}$ . We, therefore, estimate that the positive electron will obtain about  $2mc^2 Z/137$  more energy than the negative for small  $h\nu$ ; for higher  $h\nu$  the difference will be smaller.

*2. Angular Distribution.*—The average angle between the direction of motion of a created electron of energy  $E_0$  and the creating quantum is of the order  $\theta \sim mc^2/E_0$ . For large energies, therefore, the electrons are emitted mainly in the forward direction. Explicitly, the number of electrons emitted at an angle  $\theta_0$  is approximately proportional to

$$\Phi(\theta_0) d\theta_0 = \frac{\theta_0 d\theta_0}{(\Theta^2 + \theta_0^2)} , \quad \Theta = \frac{mc^2}{E_0} . \quad (60)$$

(cf. paper C, (74)). For energies of the order  $mc^2$ , the angular distribution is more complicated and the preponderance of the forward direction less marked.

*3. Total Cross-section. Comparison with Experiments.*—The total cross-section is found by integrating the cross-sections (21), (22), (36) over all possible

† For high energies  $h\nu$  the minimum  $E_0 = E_+$  is less marked than in the theory of Oppenheimer and Plesset, who obtain  $\Phi_{E+}$  proportional to  $E_0^2 + E_+^2$  which apparently is due to an error in their calculation.

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energies  $E_0$  of the negative electron. Analytical integration is possible in two cases.

(1) If  $mc^2 \ll h\nu \ll 137 mc^2 Z^{-\frac{1}{3}}$ , then formula (22) (no screening) has to be integrated, giving

$$\Phi_{\text{pair}} = r_0^2 \frac{Z^2}{137} \left( \frac{28}{9} \log \frac{2h\nu}{mc^2} - \frac{218}{27} \right), \quad (\text{no screening } h\nu \gg mc^2), \quad (61)$$

a result which has been published in the preliminary note by Heitler and Sauter (*loc. cit.*).

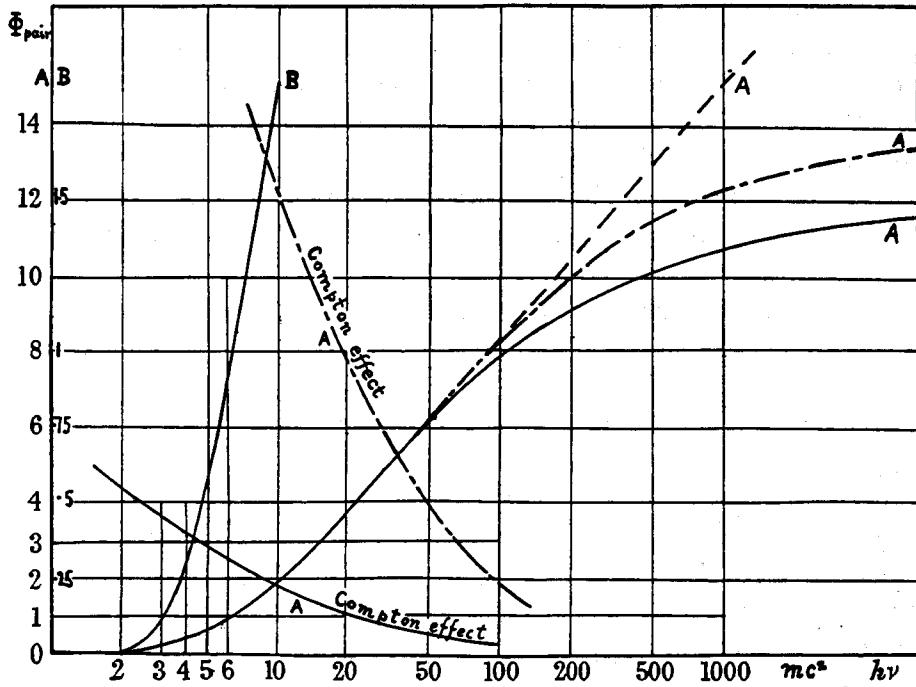


FIG. 6.—Integrated cross-section for the creation of pairs (units  $Z^2 r_0^2 / 137$ ) as a function of  $h\nu$  for lead (—),  $H_2O$  (---), and without screening (— · —). The beginning of the curve is also given with 8-fold enlargement (curve B). For comparison the cross-section for the Compton effect is given on the same scale.

(2) If  $h\nu \gg 137 mc^2 Z^{-\frac{1}{3}}$  (complete screening) we find

$$\Phi_{\text{pair}} = r_0^2 \frac{Z^2}{137} \left( \frac{28}{9} \log (183 Z^{-\frac{1}{3}}) - \frac{2}{27} \right) \quad (\text{complete screening}) \quad (62)$$

For all other values of  $h\nu$  the integration must be carried out numerically. The result is shown in fig. 6, which gives the total cross-section for the creation of pairs in lead and aluminium (units  $Z^2 r_0^2 / 137$ ). For comparison we have plotted the cross-sections for the production of Compton-electrons.

The cross-section is proportional to the square of the atomic number. It also increases rapidly with increasing energy of the quantum  $h\nu$  (for small  $h\nu$ ). For very high energies  $h\nu$  an asymptotic value is reached which is determined by the ratio of the radius of the atom to  $\hbar/mc$ . (In the space between  $\hbar/mc$  and the atomic radius the probability for the production of pairs is appreciable.)†

The calculated cross-section is in *good agreement with experiment* as regards both the absolute number of pairs produced and the dependence on energy and atomic number. The direct experiments of Curie and Joliot,‡ Blackett and Occhialini§ and others,|| give the ratio of the number of electron pairs produced by hard  $\gamma$ -rays to the number of Compton plus photo-electrons the Compton effect being calculable from the Klein-Nishina formula.¶ Table V compares the theoretical and experimental values of this ratio for lead and various quantum energies. For the theoretical values an average value of  $h\nu$  has been assumed of 3, 5.2, and 11  $mc^2$  respectively for the three sources.

Table V.—Number of Electrons Pairs produced by  $\gamma$ -rays.

Energy Source	Pb.			Al. $P_0 + Be.$	Units. $mc^2$ .
	2-4.4 Ra mixture.	5.2 ThC".	10-12 $P_0 + Be.$		
I—Theoretical cross-section for production of pairs	0.12	0.6	2.0	2.0	
II—Theoretical cross-section for production of Compton and photo-electrons	4.0	3.0	2.1	12	$Z^2 r_0^2 / 137$
III—Ratio of I to II (theoretical)	0.03	0.20	0.95	0.17	—
IV—Ratio (experimental)	(0.03)	0.22	(0.67)	(0.06)	—

The agreement is better than was to be expected. The values in brackets refer to measurements made in rather thick plates of lead, \*\* whereas the value

† Cf. § 4. This fact is in contrast to Oppenheimer and Plesset, who maintain that all pairs are produced at distances  $\hbar/mc$ .

‡ 'C. R. Acad. Sci. Paris,' vol. 196, p. 1885 (1933), and p. 1581 (1934).

§ 'Nature,' vol. 132, p. 917 (1933).

|| Grinberg, *ibid.*, vol. 197, p. 318 (1933).

¶ The number of photo-electrons is for lead roughly 10% of the number of Compton electrons, and can be calculated from Sauter's theory.

\*\* A fairly large number of positive and negative electrons is shown to be absorbed in the plate, since very often only one positron appears in the chamber without the accompanying negative electron.

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for the  $5 \cdot 2 mc^2$   $\gamma$ -radiation is reduced to infinitely thin plates.<sup>†</sup> In particular the increase of the cross-section with increasing energy is very well represented by the theory.

The dependence on the atomic number has been tested by a more indirect method by Heiting.<sup>‡</sup> He measures the "excess-scattering" of  $\gamma$ -rays in various elements (beside the Compton-scattering). This effect is known to be due to the recombination of a positive electron (after being stopped by collisions) with a negative electron, the rest energy of both electrons being emitted in two light quanta of energy  $h\nu = mc^2$  each. Since all positive electrons die after travelling a comparatively short path, the number of the emitted quanta is just twice the number of positive electrons produced. The intensity of this "scattered" radiation is found to be almost exactly proportional to  $Z^2$  over the whole range of  $Z$  from aluminium to lead (the primary radiation had an energy which was  $h\nu = 5 \cdot 2 mc^2$ ). This agreement proves the validity of Born's approximation for our calculations. This is rather surprising, since Born's approximation means an expansion in a power series in  $Ze^2/\hbar c$ .

4. *Absorption Coefficient for Light of Short Wave-length.*—If the energy of the quantum becomes high, the probability for the creation of pairs becomes larger than that for the Compton effect (see fig. 6), since the latter decreases with increasing energy as  $1/h\nu \cdot \log(2h\nu/mc^2)$ . This fact is analogous to the energy loss of particles by radiation (cf. § 6). For lead, the creation of pairs is the more probable process already for  $h\nu = 10 mc^2$ , for aluminium about  $h\nu = 35 mc^2$  is required to make the probability for the two processes equal.

The absorption of light of very short wave-length is, therefore, due to the creation of pairs rather than to the Compton effect. Since the *creation cross-section increases with increasing energy, the same is true for the absorption coefficient*, a behaviour which is rather unfamiliar. Table VI gives the absorption coefficient for hard  $\gamma$ -rays in Pb, Cu, and  $H_2O$ ; it rises, for instance, to more than  $1 \text{ cm}^{-1}$  in lead. It should, however, be considered that for  $h\nu > 137 mc^2$  the quantum theory will go wrong, as it does for the radiation of fast electrons. It is to be expected that, as a consequence, the absorption coefficient for quanta of energy greater than  $137 mc^2$  will decrease again.<sup>§</sup>

<sup>†</sup> We are indebted to Professor Blackett for his kind communication.

<sup>‡</sup> 'Z. Physik,' vol. 87, p. 127 (1933).

<sup>§</sup> [Note added in proof, May 25, 1934.—In a recently published paper v. Weizsäcker ('Z. Physik,' vol. 88, p. 612 (1934), cf. footnote<sup>†</sup> at the end §4) came to the conclusion that the theoretical results reached in this paper should be valid also for energies  $> 137 mc^2$ . If this result should be correct it would be hardly possible to reconcile it with the experiments mentioned in §7.]

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Table VI.—Absorption Coefficient for Hard  $\gamma$ -rays in various Materials in  $\text{cm}^{-1}$ .

Material.	Absorption due to	Energy in million volts.					
		5	10	20	50	100	1000
Pb .....	Compton effect....	0.235	0.141	0.082	0.039	0.022	0.003
Pb .....	Pairs .....	0.24	0.46	0.68	0.96	1.15	1.43
Pb .....	Total .....	0.48	0.80	0.76	1.00	1.17	1.43
Cu .....	Total .....	0.292	0.276	0.31	0.36	0.40	0.50
H <sub>2</sub> O .....	Total .....	0.032	0.022	0.017	0.015	0.015	0.017

### Summary.

The probability for the emission of radiation by fast electrons passing through an atom is calculated by Born's method (§ 1), the calculations going beyond previous publications mainly by considering the screening of the atomic field (§ 3). The results are discussed in §§ 5 to 7. The total radiation probability (fig. 3) becomes very large for high energies of the electron, indeed the stopping of very fast electrons (energy  $> 20 \text{ mc}^2$  for Pb) is mainly due to radiation, not to inelastic collisions. The theory does not agree with Anderson's measurements of the stopping of electrons of 300 million volts energy, thus showing that the quantum theory is definitely wrong for electrons of such high energy (§ 7) (presumably for  $E_0 > 137 \text{ mc}^2$ ).

By the same formalism, the probability for the creation of a positive and a negative electron by a  $\gamma$ -ray is calculated (§§ 2, 3). The energy distribution of the electrons is shown in fig. 5, the total creation probability in fig. 6. For  $\gamma$ -rays of  $h\nu$  between 3 and 10  $\text{mc}^2$  the theory is in very good agreement with the experiments.

## The “Neutrino”

(with R. Peierls)

*Nature* **133**, 532 (1934)

The authors show that it would be very unlikely that free neutrinos can be observed: Bethe and Peierls could not foresee that there would be nuclear reactors giving neutrino fluxes enormously greater than the radioactive sources available in 1934. Using these, Reines and Cowan (1956) were able to observe free neutrinos, work for which Reines received the Nobel Prize in 1995. Nor could they foresee accelerators giving protons of energies of  $TeV(10^{12} V)$  which produce similarly large neutrino fluxes.

## The "Neutrino"

*Nature* 133, 532

THE view has recently been put forward<sup>1</sup> that a neutral particle of about electronic mass, and spin  $\frac{1}{2}\hbar$  (where  $\hbar = h/2\pi$ ) exists, and that this 'neutrino' is emitted together with an electron in  $\beta$ -decay. This assumption allows the conservation laws for energy and angular momentum to hold in nuclear physics<sup>2</sup>. Both the emitted electron and neutrino could be described either (a) as having existed before in the nucleus or (b) as being created at the time of emission. In a recent paper<sup>3</sup> Fermi has proposed a model of  $\beta$ -disintegration using (b) which seems to be confirmed by experiment.

According to (a), one should picture the neutron as being built up of a proton, an electron and a neutrino, while if one accepts (b), the rôles of neutron and proton would be symmetrical<sup>4</sup> and one would expect that positive electrons could also sometimes be created together with a neutrino in nuclear transformations. Therefore the experiments of Curie and Joliot<sup>5</sup> on an artificial positive  $\beta$ -decay give strong support to method (b), as one can scarcely assume the existence of positive electrons in the nucleus.

Why, then, have positive electrons never been found in the natural  $\beta$ -decay? This can be explained by the fact that radioactivity usually starts with  $\alpha$ -emission and therefore leads to nuclei the charge of which is too small compared with their weight. The artificial  $\beta$ -emission was found for two unstable nuclei (most probably N<sup>13</sup> and P<sup>30</sup>) formed by capture of an  $\alpha$ -particle and emission of a neutron, and therefore having too high a charge for their mass.

A consequence of assumption (b) is that two isobares differing by 1 in atomic number can only be stable if the difference of their masses is less than the mass of electron and neutrino together. For otherwise the heavier of the two elements would disintegrate with emission of a neutrino and either a positive or negative electron. There will be only a limited region on the mass defect curve, probably at medium atomic weight, where such small differences are possible. In fact, neighbouring isobares have only been found with the mass numbers 87, 115, 121, 123, (187), (203), while isobares with atomic numbers differing by 2 are very frequent. In the first case, one of the two nuclei (Rb) is known to emit  $\beta$ -rays. In each of the last two cases one of the two isobares is stated to be exceedingly rare and its identification might be due to experimental error. The other three cases actually lie close together and have medium weight. A particular case of isobares are proton and neutron. Since all experimentally deduced values of the neutron mass lie between 1.0068 and 1.0078, they are certainly both stable even if the mass of the neutrino should be zero.

The possibility of creating neutrinos necessarily implies the existence of annihilation processes. The most interesting amongst them would be the following: a neutrino

hits a nucleus and a positive or negative electron is created while the neutrino disappears and the charge of the nucleus changes by 1.

The cross section  $\sigma$  for such processes for a neutrino of given energy may be estimated from the lifetime  $t$  of  $\beta$ -radiating nuclei giving neutrinos of the same energy. (This estimate is in accord with Fermi's model but is more general.) Dimensionally, the connexion will be

$$\sigma = A/t$$

where  $A$  has the dimension cm.<sup>2</sup> sec. The longest length and time which can possibly be involved are  $\hbar/mc$  and  $\hbar/mc^2$ . Therefore

$$\sigma < \frac{\hbar^3}{m^3 c^4 t}$$

For an energy of  $2.3 \times 10^6$  volts,  $t$  is 3 minutes and therefore  $\sigma < 10^{-44}$  cm.<sup>2</sup> (corresponding to a penetrating power of  $10^{16}$  km. in solid matter). It is therefore absolutely impossible to observe processes of this kind with the neutrinos created in nuclear transformations.

With increasing energy,  $\sigma$  increases (in Fermi's model<sup>3</sup> for large energies as  $(E/mc^2)^2$ ) but even if one assumes a very steep increase, it seems highly improbable that, even for cosmic ray energies,  $\sigma$  becomes large enough to allow the process to be observed.

If, therefore, the neutrino has no interaction with other particles besides the processes of creation and annihilation mentioned — and it is not necessary to assume interaction in order to explain the function of the neutrino in nuclear transformations — one can conclude that there is no practically possible way of observing the neutrino.

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<sup>1</sup> W. Pauli, quoted repeatedly since 1931, to be published shortly in "Rapports du Septième Conseil Solvay, Brussels", 1933.

<sup>2</sup> C. D. Ellis and N. F. Mott, *Proc. Roy. Soc.*, **A141**, 502; 1933.

<sup>3</sup> E. Fermi, *La Ricerca Scientifica*, **2**, No. 12; 1933.

<sup>4</sup> This point of view was first put forward by I. Curie and F. Joliot at the Conseil Solvay, 1933.

<sup>5</sup> I. Curie and F. Joliot, *NATURE*, **133**, 201, Feb. 10, 1934.

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## Quantum Theory of the Diplon (with R. Peierls)

*Proc. Roy. Soc. London Ser. A* **148**, 146–156 (1935)

The diplon is the heavy isotope of hydrogen, now called deuteron. It is the simplest composite nucleus. The Schrödinger equation for this 2-particle problem is solved, assuming the forces between neutron and proton are of short range, and a very simple wave function is obtained, which is today still a good approximation. The photoelectric disintegration of the deuteron is calculated; this, in fact, was the origin of the paper: James Chadwick who (with Maurice Goldhaber) had observed the photo-disintegration, challenged the authors to give a theory of the process.

## Quantum Theory of the Diplon

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### 1—INTRODUCTION

The work of Heisenberg,<sup>†</sup> Majorana,<sup>‡</sup> and Wigner<sup>§</sup> seems to show that the behaviour of protons and neutrons and their interaction in the nucleus may be described by the ordinary methods of quantum mechanics. It is of particular interest to study the simplest nuclear system, *i.e.*, the diplon, which almost certainly consists of a proton and a neutron. In dealing with such a two-body problem, the wave equation can be rigorously solved if the forces are known, and this problem therefore has the same importance for nuclear mechanics as the hydrogen atom has for atomic theory.

The force acting between a proton and a neutron has been investigated by Wigner (*loc. cit.*) who showed that in order to understand the high mass defect of  $\text{He}^4$  compared with  $\text{H}^2$  one must assume interaction forces with a range much smaller than the radius of  $\text{H}^2$ . Without knowing about these forces more than the binding energy of  $\text{H}^2$ , one can, then, investigate quantitatively the behaviour of  $\text{H}^2$  against various perturbations.

<sup>†</sup> 'Z. Physik,' vol. 77, p. 1 (1932); vol. 78, p. 156 (1932); vol. 80, p. 587 (1933).

<sup>‡</sup> 'Z. Physik,' vol. 82, p. 137 (1932).

<sup>§</sup> 'Phys. Rev.,' vol. 43, p. 252 (1933); 'Z. Physik,' vol. 83, p. 253 (1933).

2—WAVE EQUATION FOR H<sup>2</sup>

The variables of our problem are the co-ordinates of neutron and proton and the z-components of their spins. We denote by  $\psi(xs, \xi\sigma)$  the wave function for the configuration in which the proton is found at the place  $x$  with the spin  $s$  and the neutron at  $\xi$  with spin  $\sigma$ . For this function three types of wave equation have been proposed:

$$\left( \frac{\hbar^2}{2M} (\nabla_x^2 + \nabla_\xi^2) + E \right) \psi(xs, \xi\sigma) = \begin{cases} V(x - \xi) \psi(xs, \xi\sigma) & (1A) \\ V(x - \xi) \psi(\xi\sigma, xs) & (1B) \\ V(x - \xi) \psi(\xi s, x\sigma) & (1C) \end{cases}$$

where  $M$  is the mass of one proton, which is, in sufficient approximation, equal to that of the neutron. Equation (1A) (ordinary interaction force) was discussed by Wigner (*loc. cit.*) who showed that it can describe correctly the behaviour of the nuclei up to He<sup>4</sup>. It does not explain, however, the fact that the addition of more particles does not increase the mass defect per particle (*cf.* Majorana, *loc. cit.*). In order to explain this fact one has to assume a force of an exchange type leading to saturation, the simplest forms of which are (1B) and (1C). (1B) was proposed by Heisenberg, but it leads to saturation for the H<sup>2</sup> nucleus already and therefore must lead to too low a mass defect for He<sup>4</sup>. The equation (1C) proposed by Majorana, leads to He<sup>4</sup> as a saturated configuration, and therefore seems to fulfil all requirements. We shall in the following adopt (1C), but we shall see that our results for the behaviour of the diplon at not too high energies are practically independent of this assumption.

The solution of (1) will be of the form

$$\psi(xs, \xi\sigma) = \chi\left(\frac{x+\xi}{2}\right) \alpha(s\sigma) \phi(x - \xi), \quad (2)$$

$$\phi(x - \xi) = u(r) P_{lm}(\theta\phi) \quad (2A)$$

where  $r = |\mathbf{r}|$  is the distance between the points  $x$  and  $\xi$ ;  $\theta\phi$  the direction of the vector  $\mathbf{r}$  and  $P_{lm}$  a spherical harmonic. Then  $u$  must satisfy the equation

$$\frac{\hbar^2}{M} \left( \frac{1}{r} \frac{d^2}{dr^2} (ru) - \frac{l(l+1)}{r^2} u \right) + Eu = (-1)^l V(r) u. \quad (3)$$

For a fixed value of  $l$ , this equation is equivalent to an ordinary

Schrödinger equation, the only difference against (1A) being that the "potential" is attractive for even and repulsive for odd values of  $l$ . If we had adopted (1B) the sign of the potential would also differ for the triplet and singlet state.

The function  $V$  has been investigated by Wigner who showed that  $V$  has appreciable values only if  $r < a \approx 1.0 \cdot 10^{-13}$  cm and at smaller distances becomes of the order  $10^8$  volts.<sup>†</sup> Wick<sup>‡</sup> tried to determine  $V$  from the mass defects of heavy nuclei with the aid of (1C). The form of  $V$  obtained in this way is in reasonable agreement with that of Wigner.

In solving the equation for  $l = 0$ , one can therefore at small distances neglect the energy compared with the potential, so that the phase  $= \frac{1}{ru} \frac{d(ru)}{dr}$  of the wave function will have a definite value  $\alpha$  at distances small compared with the wave-length, but larger than  $a$ . Thus one can, instead of solving equation (3), work with the equation for free motion, but with the boundary condition that

$$-\frac{1}{ru} \frac{d(ru)}{dr} \rightarrow \alpha \quad \text{for } r = 0.$$

The value of  $\alpha$  can be deduced from the mass defect of  $H^2$ .

For  $l \neq 0$ , the potential  $V$  will have no appreciable effect at all, because the centrifugal force makes the wave function very small for distances small compared with the wave-length and the potential at still smaller distances will therefore not matter.<sup>§</sup>

If, therefore, (i) the wave-length of the particles is large compared with  $a$ , and (ii) their relative energy small compared with the values of

<sup>†</sup> The arguments of Wigner are based on (1A), but just because the range of the forces turns out so very small, the same results may be deduced, without appreciable modification, from (1C) as well. The reason is, that over the distances where  $V(x - \xi)$  is different from zero, the wave function varies slowly and  $\psi(x\xi)$  and  $\psi(\xi x)$  are nearly equal, unless  $\psi$  has a node at the point  $x = \xi$  which, however, for the nuclei up to  $He^4$  will not occur.

<sup>‡</sup> 'Nuovo Cim.', vol. 11, p. 227 (1934).

<sup>§</sup> The very short range of the interaction forces between neutron and proton leads to consequences for the scattering of slow neutrons by protons which have been discussed by Wigner (*loc. cit.*) and Wick ('Z. Physik,' vol. 84, p. 799 (1934)) and *loc. cit.* These authors have pointed out that observations of very fast neutrons would afford a means for both estimating the range of the forces and deciding directly between equations (1A, B, C). The mathematical treatment for high energies given in these papers is, however, not quite complete and we hope to come back to this question in a later publication.

$V$  at small distances (these two conditions are equivalent) one can replace the solution of (3)

for  $l \neq 0$  by wave functions of free particles,  
for  $l = 0$  by solutions of

$$\frac{\hbar^2}{M} \frac{1}{r} \frac{d^2}{dr^2} (ru) + Eu = 0, \quad (4)$$

with the boundary condition

$$\left( -\frac{1}{ru} \frac{d(ru)}{dr} \right)_{r=0} = \alpha. \quad (5)$$

Under these assumptions, there is only one discrete state with  $l = 0$  and the wave function

$$u_0 = \frac{C}{r} e^{-\alpha r}. \quad (6)$$

The condition of normalization determines  $C$ :

$$C = \sqrt{\alpha/2\pi}. \quad (7)$$

The corresponding energy is

$$-\epsilon = -\frac{\hbar^2}{M} \alpha^2, \quad (8)$$

and  $\alpha$  has to be so determined as to make  $\epsilon$  equal to the binding energy of  $H^3$ . This energy has recently been determined fairly accurately by Chadwick† and was found to be

$$\epsilon = 2 \cdot 1 \cdot 10^4 \text{ volts},$$

which gives

$$\alpha = 2 \cdot 2 \cdot 10^{12} \text{ cm}^{-1},$$

$1/\alpha$  is indeed much larger than the assumed range of the interaction forces.

### 3—ABSORPTION OF $\gamma$ -RAYS BY DIPLONS

If a  $\gamma$ -ray of energy  $h\nu$  falls on a diplon it may be absorbed, producing a proton and a neutron. This process is analogous to the photo-electric effect of an atom and the effective cross section is given by the well-known formula‡

$$\sigma = \frac{8\pi^2 e^2 v}{c} |z_{0K}|^2, \quad (9)$$

† Chadwick and Goldhaber, 'Nature,' vol. 134, p. 237 (1934).

‡ Cf., e.g., Kemble and Hill ('Rev. mod. Phys.', vol. 2, p. 11 (1930)) formula (28). This formula differs from (9) by a factor  $h^3 v/c$ , because the authors calculate the ratio of transition probability and radiation density per unit frequency instead of the cross-section per unit energy.

where  $e$  is the protonic charge,  $c$  the velocity of light and

$$z_{0k} = \int u_0 \frac{1}{2} z \phi_k d\tau. \quad (10)$$

Here  $u_0$  is given by (6),  $z$  is the  $z$ -component of  $r$ , and  $\frac{1}{2}z$  consequently the  $z$ -co-ordinate of the proton with respect to the centre of gravity.  $\phi_k$  is the wave function of a state with the energy  $E = h\nu - e$  normalized in energy scale. Of all possible states with this energy, only that belonging to  $l = 1$  gives a non-vanishing matrix element (10). The corresponding wave function is then, as we have seen, identical with the wave function for free motion. If, on the other hand, we insert in (10) all wave functions of free motion with energy  $E$ , again only that with  $l = 1$  gives a non-vanishing integral. We are therefore allowed to use wave functions for free motion in Cartesian co-ordinates :

$$\phi_k = (2\pi)^{-3/2} e^{i(\mathbf{k} \cdot \mathbf{r})} \quad (11)$$

(11) is normalized in wave vector scale. In order to obtain energy normalization we have to add a factor

$$k^3 \frac{dk}{dE} d\Omega = \frac{Mk}{2\hbar^3} d\Omega,$$

where  $d\Omega$  is the element of the direction of motion, and the reduced mass  $M/2$  enters instead of  $M$  as we are concerned with the relative motion. Thus in (9) we may write

$$|z_{0k}|^2 = \frac{1}{(2\pi)^3} \frac{Mk}{2\hbar^3} \int d\Omega |z_{0k}|^2, \quad (12)$$

where

$$z_{0k} = \int d\tau u_0 \frac{1}{2} z e^{i(\mathbf{k} \cdot \mathbf{r})}. \quad (13)$$

The length of  $k$  is defined by

$$\hbar^3 k^3 = p^3 = M(h\nu - e). \quad (14)$$

Inserting (6) the matrix element becomes

$$z_{0k} = \frac{1}{2} \sqrt{\frac{\alpha}{2\pi}} \frac{1}{i} \frac{\partial}{\partial k_s} \int d\tau \frac{1}{r} e^{-ar + ik_r \cos \theta},$$

where  $\theta$  is the angle between  $k$  and  $r$ .

$$z_{0k} = -4\pi i \sqrt{\frac{\alpha}{8\pi}} \frac{\partial}{\partial k_s} \left( \frac{1}{\alpha^3 + k^3} \right) = i \sqrt{2\pi\alpha} \frac{2k_s}{(\alpha^3 + k^3)^2}$$

Inserting this into (12) we obtain

$$|z_{0E}|^2 = \frac{2}{3\pi} \frac{M}{\hbar^2} \frac{\alpha k^3}{(\alpha^2 + k^2)^4}, \quad (15)$$

and from (9):

$$\sigma = \frac{16\pi^2}{3} \frac{Me^3 v \alpha k^3}{\hbar^2 c (\alpha^2 + k^2)^4}.$$

Expressing now  $\alpha$  and  $k$  from (8) and (14):

$$\begin{aligned} \sigma &= \frac{16\pi^2}{3} \frac{\hbar^2 e^2 v (hv - \epsilon)^{3/2} \epsilon^{1/2}}{Mc (hv)^4}, \\ \sigma &= \frac{8\pi}{3} \frac{e^2}{\hbar c} \frac{1}{\alpha^2} \frac{(\gamma - 1)^{3/2}}{\gamma^3}, \end{aligned} \quad (16)$$

where

$$\gamma = hv/\epsilon. \quad (17)$$

With the estimated value of  $\alpha$  given above†

$$\sigma \approx 1.25 \cdot 10^{-26} (\gamma - 1)^{3/2} \gamma^{-3} \text{ cm}^2.$$

This becomes a maximum for  $\gamma = 2$  where  $\sigma = 1.6 \cdot 10^{-27} \text{ cm}^2$ .

#### 4—CAPTURE OF NEUTRONS BY PROTONS

The inverse process to the one considered in the last section is the formation of a diplon from the separate particles under emission of  $\gamma$ -rays. The probability  $P_{12}$  of this process is connected with that  $P_{21}$  for the inverse in the following way:

$$P_{12}/g_2 = P_{21}/g_1,$$

where  $g_1$  and  $g_2$  are the statistical weights of the final states of the system.

The number of states per unit momentum vector is the same for both particles and light quanta. The number of states for the relative motion per unit energy is proportional to

$$\frac{p^3 dp}{dE} = \frac{Mp}{2},$$

† The experimental value given by Chadwick ('Nature,' vol. 134, p. 237, August 18, 1934) is only  $10^{-28} \text{ cm}^2$ . This would agree with (16) only if  $\gamma - 1 = 0.04$ , i.e., if by accident the energy of the  $\gamma$ -rays employed was only just above the limit of absorption. Whether this is actually so or whether (16) is actually too large can only be decided by further experiments.

where  $p = \frac{1}{2}Mv$  is the momentum in the co-ordinate system where the centre of gravity is at rest. For the light quantum we have instead

$$\frac{(hv/c)^3 d(hv/c)}{d(hv)} = \frac{(hv)^3}{c^3},$$

and additional factor 2 for polarization.

Therefore the ratio of the probabilities for capture and absorption will be†

$$\frac{4(hv)^3}{c^3 Mp}$$

if the density of the incident particles is the same. In order to obtain the cross-section we must compare the yield not for equal density but for equal current and so must add a factor  $c/v$ , where  $v$  is the velocity of the incident neutron. Thus if  $\sigma$  is the cross-section (16) the cross-section for capture becomes

$$\begin{aligned}\sigma' &= 2 \frac{(hv)^3}{c^3 p^3} \sigma = 2 \frac{(hv)^3}{Mc^4 (hv - \epsilon)} \sigma \\ \sigma' &= 2 \frac{\epsilon}{Mc^2} \frac{\gamma^2}{\gamma - 1} \sigma\end{aligned}\quad (18)$$

or

$$\sigma' = \frac{16\pi}{3} \frac{e^2}{\hbar c} \left( \frac{\hbar}{Mc} \right)^2 \frac{(\gamma - 1)}{\gamma} \sigma^{1/2} \quad (18A)$$

(18A) is again a maximum for  $\gamma = 2$ , i.e., if the energy of the incident neutron is  $\epsilon$  in the relative co-ordinate system, i.e.,  $2\epsilon$  in the system where the proton is at rest. Then

$$\sigma' = 2 \cdot 70 \cdot 10^{-29} \text{ cm}^2.$$

The capture therefore seems hardly observable.

Instead of being captured, the neutron passing through hydrogen may, of course, radiate only part of its energy, but the cross-section for this process is only of the same order of magnitude.

† This ratio involves the assumption that proton and neutron can be bound together also if their spins are antiparallel and that the probability of capture does not depend on the relative spin directions. The assumption is correct if the model of either Wigner or Majorana is assumed and the magnetic force between the spins is considered as a small perturbation. In Heisenberg's model there would be no bound singlet state, the cross-section for capture would then be reduced by a factor  $\frac{1}{2}$ .

5—SCATTERING OF  $\gamma$ -RAYS BY DIPLONS

$\gamma$ -rays affect both the relative co-ordinate and the centre of gravity of the diplon. The latter gives the classical scattering according to Thomson's formula, while the inner degree of freedom gives an additional scattered wave which may easily be calculated from the Heisenberg-Kramers formula, using the matrix elements (15).†

The total nuclear scattering per unit solid angle under an angle  $\theta$  then becomes :

$$\left\{ \frac{1}{2} \frac{e^2}{Mc^2} \frac{1}{\gamma^2} (4 + 3\gamma^2 - 2(1 + \gamma)^{3/2} - 2(1 - \gamma)^{3/2}) \right\}^2 \frac{1}{2} (1 + \cos^2 \theta),$$

if  $\gamma < 1$ , and

$$\left\{ \frac{1}{2} \frac{e^2}{Mc^2} \frac{1}{\gamma^2} (4 + 3\gamma^2 - 2(1 + \gamma)^{3/2}) \right\}^2 \frac{1}{2} (1 + \cos^2 \theta) \quad (19)$$

if  $\gamma > 1$ , where again  $\gamma = h\nu/e$ .

The scattering is always smaller than that of a free proton and becomes equal to the latter only for  $\gamma \gg 1$ . The order of magnitude of this effect is therefore extremely small, corresponding to a total cross-section of about  $2 \cdot 10^{-31} \text{ cm}^2$ , so that it is practically impossible to observe it.

## 6—DISINTEGRATION OF DIPLONS UNDER ELECTRON BOMBARDMENT

If fast electrons of momentum  $P$  and energy  $W$  strike a diplon, they may be scattered through an angle  $\theta$  and afterwards have a smaller energy  $W'$  (momentum  $P'$ ), while the energy difference serves to disintegrate the diplon. The calculation of the probability is very similar to the disintegration by a light wave (*cf.* section 3). Instead of the light wave one has to insert the electromagnetic field belonging to the transition of the electron from  $P$  to  $P'$ .‡ If  $\Psi_p$  and  $\Psi_{p'}$  are initial and final wave function of the electron, the field derives from the four-potential :

$$\begin{aligned} \Phi_0 &= \frac{4\pi e\hbar^2 (\Psi_{p'}^* \Psi_p)}{(P - P')^2 - (W - W')^2/c^2} = 4\pi e\hbar^2 c^3 a_0 \frac{\exp(i(qr)/hc)}{q^2 - (W - W')^2} \\ \Phi_k &= \frac{4\pi e\hbar^2 (\Psi_{p'}^* \alpha_k \Psi_p)}{(P - P')^2 - (W - W')^2/c^2} = 4\pi e\hbar^2 c^3 a_k \frac{\exp(i(qr)/hc)}{q^2 - (W - W')^2} \quad (20) \\ &\quad (k = 1, 2, 3). \end{aligned}$$

† Cf. e.g., Kemble and Hill, *loc. cit.*, p. 22, equation (61).

‡ Chr. Möller, 'Z. Physik,' vol. 70, p. 786 (1931).

Here  $\alpha_k$  are Dirac's matrices,  $a_0$  and  $a_k$  are constants arising from the ratios of the components of the Dirac wave functions  $\Psi_P$  and  $\Psi_{P'}$ . They depend upon  $P$  and  $P'$  and upon the spin directions.  $q/c = P - P'$  is the momentum difference between initial and final electronic state. If we consider (20) as a perturbation acting on the diplon, the transition probability is proportional to the square of the matrix element

$$\int u_0 \exp(\frac{1}{2}i(qr)/\hbar c) (a_0 - \sum_k a_k v_k/c) \phi_E d\tau. \quad (21)$$

Here  $v_k = \frac{\hbar}{iM} \frac{\partial}{\partial r_k}$  is the operator of the proton velocity and  $\frac{1}{2}r$  in the exponent is again its distance from the centre of gravity.  $qr/\hbar c$  is small compared with unity over the region where  $\phi_0 \neq 0$  unless  $2W \sin \frac{1}{2}\theta$  becomes of the order  $4 \cdot 10^7$  volts. Usually, therefore, it is sufficient to expand the exponential, retaining only the constant term where it is multiplied by  $v$  and the linear, multiplied by  $a_0$ . After averaging over the spin directions of the electron the differential cross-section becomes :

$$\begin{aligned} \sigma_{0E} dE d\Omega = 4 \left( \frac{e^2}{\hbar c} \right)^2 \frac{P'}{P} \frac{|z_{0E}|^2}{[q^2 - (W - W')^2]^2} & [(q^2 - (W - W')^2)(W^2 + W'^2) \\ & - \frac{1}{2}(q^2 - (W - W')^2)^2 - \frac{1}{2}m^2c^4(W - W')^2] dE d\Omega, \end{aligned} \quad (22)$$

Integration with respect to all directions of the scattered electron gives

$$\sigma_{0E} dE = 8\pi \left( \frac{e^2}{\hbar c} \right)^2 |z_{0E}|^2 \left\{ \frac{W^2 + W'^2}{c^2 P^2} \log \frac{WW' + c^2 PP' - m^2 c^4}{(W - W') mc^2} - \frac{1}{2} \frac{P'}{P} \right\} dE, \quad (23)$$

$z_{0E}$  is the matrix element (15).

The total cross-section  $\sigma_D$  is given by the integral of (23) over the range  $0 < E < W - mc^2 - \epsilon$ .  $|z_{0E}|^2$  decreases rapidly at high energies  $E$  and we may therefore assume  $W' = W$  except in the denominator  $W - W' = E + \epsilon$ , if  $W$  is large compared with  $\epsilon$ . We may then also write  $W$  instead of  $cP$  and integrate from 0 to  $\infty$ . Then the total cross-section will be

$$\sigma_D = 16\pi \left( \frac{e^2}{\hbar c} \right)^2 \int_0^\infty dE |z_{0E}|^2 \left\{ \log \frac{2W^2}{(E + \epsilon) mc^2} - \frac{1}{2} \right\}. \quad (24)$$

We may define an average excitation energy  $A$  by putting (cf. (15))

$$\log \frac{A}{\epsilon} = \frac{\int_0^\infty dE |z_{0E}|^2 \log(E + \epsilon/\epsilon)}{\int_0^\infty dE |z_{0E}|^2} = \frac{\int_1^\infty d\gamma (\gamma - 1)^{1/2} \gamma^{-4} \log \gamma}{\int_1^\infty d\gamma (\gamma - 1)^{1/2} \gamma^{-4}}, \quad (25)$$

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where

$$\gamma = (E + \epsilon)/hv,$$

and with this notation  $\sigma_0$ , becomes:

$$\begin{aligned}\sigma_D &= 16\pi \left(\frac{e^2}{hc}\right)^2 \int_0^\infty |z_{0K}|^2 dE \left\{ \log \frac{2W^2}{\epsilon mc^2} - \frac{1}{4} \right\}, \\ &= 16\pi \left(\frac{e^2}{hc}\right)^2 (z^2)_0 \left\{ \log \frac{2W^2}{\epsilon mc^2 A} - \frac{1}{4} \right\}. \quad (26)\end{aligned}$$

Here we have used the fact that  $\int_0^\infty dE |z_{0K}|^2$  is the diagonal matrix element of  $z^2$  for the ground state, which is

$$(z^2)_0 = \int u_0^2 \left(\frac{z}{2}\right)^2 d\tau = \frac{1}{2} \int u_0^2 r^2 d\tau = \frac{1}{24\alpha^2} \quad (27)$$

(cf. (10), (6)). The numerical evaluation of (25) yields

$$\log \frac{A}{\epsilon} = 1.375,$$

and therefore

$$\sigma_D = \frac{2\pi}{3\alpha^2} \left(\frac{e^2}{hc}\right)^2 \left\{ \log \frac{W^2}{\epsilon mc^2} - 1.432 \right\}. \quad (28)$$

This, assuming the value for  $\alpha$  given in section 2, yields

$$\sigma_D = 2.3 \cdot 10^{-29} \left\{ \log \frac{W^2}{\epsilon mc^2} - 1.432 \right\} \text{ cm}^2.$$

The probability of the process per centimetre path in heavy water will then be

$$1.5 \cdot 10^{-6} \left\{ \log \frac{W^2}{\epsilon mc^2} - 1.432 \right\}$$

for  $W = 10^3$  volts,  $\log(W^2/\epsilon mc^2) \sim 9.2$ , the process will therefore occur once in 0.8 km of path. This seems difficult, but not absolutely impossible to observe. The produced neutrons will have kinetic energies of the order  $3\epsilon$ .

At lower energies, the integral of (23) decreases rapidly, and if the available energy  $W - \epsilon - mc^2$  is small, the total cross-section becomes proportional to  $(W - \epsilon - mc^2)^3$ .

## 7—LIMITATIONS OF THE EMPLOYED MODEL

The approximations we have made consisted in assuming (i) that  $u_0$  has the form (6) throughout, while it actually will differ from (6) for

radii of the order  $a \sim 10^{-13}$  cm, and reach a finite value for  $r = 0$ ; (ii) that the functions for  $l \neq 0$  are solutions of the field-free equation while actually at radii smaller than  $a$  they are subject to a strong attracting (for even  $l$ ) or repelling (odd  $l$ ) force.

The actual wave functions will, therefore, give values for  $z_{0E}$  which for small  $E$  differ from our approximation by a relative amount of the order  $\alpha a$ , while for  $E \sim 10^6$  volts,  $|z_{0E}|^2$  may differ appreciably from our result. Since, however, in sections 3 and 4  $|z_{0E}|^2$  enters only for small  $E$ , and in 5 and 6 the large values of  $E$  give no appreciable contribution to the integrals, our results can only be wrong by  $\alpha a$  which is about 15%. An estimate of the influence of the neglect shows that for small energies the deviations for  $l = 1$  have no importance, while that for the ground state tends to increase the matrix element slightly. This latter fact shows that the results are even to a higher approximation independent of whether one assumes equation (1A) or (1B) instead of (1C).

Equations (1A) and (1C) lead to a solution for the ground state whether the spins of proton and neutron are parallel or antiparallel. By taking into account magnetic interaction forces one could obtain a splitting into two levels, which would give rise to a discrete  $\gamma$ -absorption line. It seems impossible to treat this problem with the present theoretical means.

The authors wish to express their thanks to Dr. J. Chadwick for discussion of his experiments which led to these considerations. Their thanks are also due to Manchester University and in particular to Professor W. L. Bragg for their hospitality.

#### SUMMARY

It is shown that our present knowledge of the intra-nuclear forces allows us to make definite predictions for the behaviour of the diplon. According to these calculations the cross-section for disintegration of a diplon by absorption of  $\gamma$ -rays is of the order  $10^{-27}$  cm $^2$ , § 3. In addition the cross-sections for capture of neutrons by protons, § 4, for scattering of  $\gamma$ -rays, § 5, and disintegration by electron bombardment, § 6, have been calculated.

## The Scattering of Neutrons by Protons

(with R. Peierls)

*Proc. Roy. Soc. London Ser. A* **149**, 176–183 (1935)

This is a sequel to the previous paper. Assuming short range forces, it is shown that the scattering is isotropic at energies up to more than 10 MeV. The cross section for low neutron energies,  $E_0 \ll \epsilon$ , the deuteron binding energy, is calculated to be 2.4 barns. Subsequent experiments showed that the cross section is actually about 10 times larger: this was explained by E. Wigner as being due to the existence of a  $^1S$  state of the deuteron. This suggestion was confirmed by experiment, and it was shown that the  $^1S$  state is virtual.

## The Scattering of Neutrons by Protons

By H. A. BETHE and R. PEIERLS, University of Manchester

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I. The mass defects of the lightest nuclei, particularly the ratio between that of the diplon and the  $\alpha$ -particle, make it very probable that the range of the interaction force between proton and neutron is very small, of the order of about  $10^{-13}$  cm.\* Therefore, in all experiments in which scattering of neutrons by protons has been observed, their wave-length is larger than the range of the interaction force. In these circumstances it is well known that the scattering intensity will be independent of angle for that co-ordinate system in which the centre of gravity is at rest.<sup>†</sup> For much higher energies, of course, this will no longer be true and one will expect then an anisotropy in the scattered intensity. This effect will become appreciable for energies for which the wave-length is of the same order as the range of the forces. Exact measurements of the angular distribution of scattered fast neutrons would therefore afford a direct check of the assumption of a short range and an estimate of this range. The existing experiments<sup>‡</sup> show an isotropic scattering within

\* Wigner, 'Phys. Rev.', vol. 43, p. 252 (1933).

† Wigner, 'Z. Physik,' vol. 83, p. 253 (1933); Chadwick, 'Proc. Roy. Soc.,' A, vol. 142, p. 1 (1933).

‡ Chadwick, *loc. cit.*; Auger and Monod-Herzen, 'C. R. Acad. Sci., Paris,' vol. 196, p. 1102 (1933); Kurie, 'Phys. Rev.,' vol. 43, p. 672 (1933).

the limits of error, but are not accurate enough to allow very definite conclusions.

2. The importance of such experiments is further increased by the fact that, as was pointed out by Wick,\* the sign of the asymmetry in the scattering depends on whether the interaction is of the ordinary type or an exchange force as proposed by Heisenberg† and Majorana,‡ and observations of the asymmetry could therefore decide this question.

For very high energies of the scattered particles (wave-length small compared with range) for "ordinary" forces§ this asymmetry is always such that most of the particles are scattered through small angles (*i.e.*, most of the observed protons move at right angles to the incident neutron beam). For exchange forces one gets the opposite behaviour, *i.e.*, the neutrons will preferentially be scattered backwards in the co-ordinate system of relative motion (in the ordinary co-ordinate system the protons will then mostly go forward). This behaviour can be interpreted as the incident particle going on with a small deflection, but in the process of scattering it has changed role with the scattering particle and has become a proton.

It has been tacitly assumed that this will be quite generally true and that a forward maximum in the scattering will always indicate ordinary forces, while a backward maximum would require exchange.

We shall show, however, that just for the proton-neutron interaction this assumption fails for not very high energies. For these we just get a backward maximum with ordinary and a forward maximum with exchange forces, whereas the effect reverses its sign at a certain rather high energy.|| This behaviour is closely connected with the fact that the interaction forces admit a state in which the particles are bound together, as we know from the existence of the dipion.

3. In the following we denote by  $r$  the length of the radius vector between proton and neutron and by  $\theta$  its angle with the incident beam, by  $E, v, k$  the energy, velocity and wave number of the incident neutrons in the relative co-ordinate system and by  $E_0, v_0, k_0$  the same quantities for the system where the proton is initially at rest.

\* 'Z. Physik,' vol. 84, p. 799 (1933).

† 'Z. Physik,' vol. 77, p. 1 (1932).

‡ 'Z. Physik,' vol. 82, p. 137 (1933).

§ We use here and subsequently the word "ordinary" forces as distinct from exchange forces, for interactions corresponding to wave mechanical operators that do not interchange the co-ordinates of protons and neutrons.

|| The calculations of Wigner ('Z. Physik,' *loc. cit.*) led to different results, but they contained an error in the rather complicated analysis.

$M$  is the mass of the proton or the neutron,  $V(r)$  the interaction potential, which for definiteness we first suppose to be an "ordinary" one, and  $\epsilon$  the binding energy of the dipion.

The Schrödinger equation then separates in polar co-ordinates; we write

$$r\psi = \sum_l u_l(r) P_l(0), \quad (1)$$

where  $P_l$  is the spherical harmonic of order  $l$  and  $u_l$  has to satisfy the equation\*

$$\frac{\hbar^2}{M} \left( \frac{d^2 u_l}{dr^2} - \frac{l(l+1)}{r^2} u_l \right) + (E - V(r)) u_l = 0, \quad (2)$$

and asymptotically for large  $r$  has the form

$$u_l = \text{const. } \sin(kr - \frac{1}{2}l\pi + \delta_l). \quad (3)$$

The phases  $\delta_l$  have to be determined by integration of (2). Then the effective cross-section for scattering through an angle  $\theta$  becomes†

$$d\sigma = \frac{\pi}{2k^2} \left| \sum_l (2l+1) P_l(0) (e^{2i\delta_l} - 1) \right|^2 \sin \theta \, d\theta. \quad (4)$$

We now assume  $V$  to have a range of order  $a$  which is small compared with the wave-length  $\lambda = 1/k$ . In this case all phases  $\delta_l$  will be small except for  $l=0$ , because the centrifugal force  $\hbar^2 l(l+1)/Mr^2$  already makes the eigen-function very small for radii  $r < l\lambda$ .

4. We begin with the discussion of  $\delta_0$ . We know of the potential  $V$  that the equation (2<sub>0</sub>) admits a solution with a negative energy, viz.,  $-\epsilon$ . There will be only one negative eigen-value, because the difference between the levels must be of the order  $\hbar^2/Ma^2$  which with the assumed value of  $a \sim 10^{-13}$  cm becomes of the order  $10^4$  volts. The eigen-function  $u_0$  belonging to this bound state will increase quickly for  $r < a$ , and for large  $r$  will show a slow exponential drop,‡ of the form

$$\left. \begin{aligned} u_0 &= \text{const. } e^{-\alpha r} \\ \alpha &= \sqrt{M\epsilon/\hbar^2} \sim 2 \cdot 3 \cdot 10^{12} \text{ cm}^{-1} \end{aligned} \right\}. \quad (5)$$

In the transitional region  $r \sim a$  the expression  $\frac{1}{u_0} \frac{du_0}{dr}$  must therefore be slightly negative and of the order  $-\alpha$ .

\*  $\frac{1}{2}M$  = reduced mass.

† Mott and Massey, "Atomic Collisions," Oxford Press, 1933, p. 24.

‡ Bethe and Peierls, 'Proc. Roy. Soc.,' A, vol. 148, p. 146 (1935).

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If we now consider a small positive energy, the value of  $\frac{1}{u_0} \frac{du_0}{dr}$  for  $r = a$  will be practically the same as for the small negative energy  $-\epsilon$ . This can be shown in the following way: by writing (2<sub>0</sub>) for two different values of E one can easily derive the following relation for the corresponding wave functions  $u_0$  and  $u'_0$ :

$$\left[ u_0 \frac{du'_0}{dr} - u'_0 \frac{du_0}{dr} \right]_{r=a} = \frac{M}{\hbar^2} (E - E') \int_0^a u_0 u'_0 dr. \quad (6)$$

If the difference  $E - E'$  is small, we have

$$\frac{d}{dE} \left( \frac{1}{u_0} \frac{du_0}{dr} \right)_{r=a} = - \frac{M}{\hbar^2} \frac{1}{u_0^2(a)} \int_0^a u_0^2(r) dr. \quad (7)$$

The integral on the right-hand side is of the order  $au_0^2(a)$ . It actually is somewhat smaller, since  $u_0^2(r)$  vanishes at  $r = 0$  and its value at  $r = a$  is practically equal to its maximum value. Therefore

$$\left( \frac{1}{u_0} \frac{du_0}{dr} \right)_{r=a} \sim -\alpha - (E + \epsilon) \frac{\gamma Ma}{\hbar^2}; \quad 0 < \gamma < 1. \quad (8)$$

For the special case of a potential hole of rectangular shape, we find  $\gamma = \frac{1}{2}$ . The right-hand side of (8) differs appreciably from  $\alpha$  only if

$$E \sim \frac{\hbar^2 \alpha}{Ma} = \sqrt{\epsilon \cdot \frac{\hbar^2}{Ma^2}}, \quad (9)$$

which is of the order  $1 \times 10^7$  volts (corresponding to a neutron energy  $E_0 = 2 \times 10^7$  volts).

If, therefore, the energy is smaller than (9) we have essentially

$$\left( \frac{1}{u_0} \frac{du_0}{dr} \right)_a = -\alpha,$$

and since  $u_0$  will already have the form (3<sub>0</sub>) for  $r = a$ , we see that

$$k \frac{\cos(ka + \delta_0)}{\sin(ka + \delta_0)} = -\alpha, \quad (10)$$

which yields

$$\begin{aligned} \delta_0 &= -ka + \operatorname{tg}^{-1}(-k/\alpha) \\ &= \pi/2 + \operatorname{tg}^{-1}(\alpha/k) - ka. \end{aligned}$$

According to (4) the differential and total cross-sections then become

$$\left. \begin{aligned} d\sigma &= \frac{2\pi}{\alpha^2 + k^2} \sin \theta d\theta \\ \sigma &= \frac{4\pi}{\alpha^2 + k^2} = 24 \times 10^{-25} \frac{\epsilon}{\epsilon + \frac{1}{2}E_0} \text{ cm}^2 \end{aligned} \right\}, \quad (11)$$

where  $E_0 = 2E$  is the energy of the incident neutron and  $\epsilon = 2 \cdot 2 \cdot 10^6$  volts.

The cross-section (11) is rather larger than the experimental values of Chadwick. For  $E_0 = 4 \cdot 3 \cdot 10^6$  volts ( $v = 2 \cdot 9 \cdot 10^7$  cm/sec) Chadwick finds a cross-section between  $5$  and  $8 \times 10^{-25}$  cm<sup>2</sup> (radius 4 to  $5 \times 10^{-13}$ ), whereas (11) gives  $12 \times 10^{-25}$ ; for  $E_0 = 2 \cdot 1 \times 10^6$  volts ( $v = 2 \cdot 10^7$  cm/sec) the corresponding figures are  $11$  to  $15 \times 10^{-25}$  (experimental) and  $16 \times 10^{-25}$  (theoretical). Considering the very indirect experimental method the agreement can, however, be considered as fair.

The assumption of a short range for the potential can thus be checked both by the isotropy and by the absolute magnitude of the cross-section (11).

For energies that are small compared with (9),  $\delta_0$  is larger than  $\pi/2$  since  $k^2 \ll \alpha/a$ , but above a certain energy of the order (9),  $\delta_0$  will become smaller than  $\pi/2$ . In order to see this we remark that  $\delta_0 = \pi/2$  is equivalent to

$$\left( \frac{1}{u_0} \frac{du_0}{dr} \right)_a = -k \operatorname{tg} ka \sim -k^2 a,$$

and according to (8)

$$\text{i.e., } -\alpha - (E + \epsilon) \gamma Ma/\hbar^2 = -\alpha - \gamma a (k^2 + \alpha^2) = -k^2 a,$$

$$k^2 (1 - \gamma) = \alpha/a - \alpha^2 \gamma$$

$$E_* = \frac{1}{1 - \gamma} \sqrt{\epsilon \frac{\hbar^2}{Ma^2}}. \quad (12)$$

Since  $1 - \gamma$  is positive and of order unity this energy is of the order (9).

5. For the evaluation of  $\delta_1$ , we compare the behaviour of the function  $u_1$  and the function  $w_1$  that is a solution of (2<sub>1</sub>) when  $V$  is put equal to zero. One easily derives that

$$(w_1 \frac{du_1}{dr} - u_1 \frac{dw_1}{dr})_{r=R} = \frac{M}{\hbar^2} \int_R^\infty V(r) u_1(r) w_1(r) dr,$$

where  $R$  is an arbitrary large distance. Inserting (3<sub>1</sub>), we find

$$-ig(kR + \delta_1) + igkR = \frac{M}{\hbar^2 k} \frac{1}{u_1(R) w_1(R)} \int_R^\infty V u_1 w_1 dr.$$

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It is convenient to choose such a distance  $R$  that  $ig kR = 0$ , then  $w_1(R)$  has just its relative maximum value and

$$ig \delta_1 = - \frac{M}{\hbar^2 k u_1(R) w_1(R)} \int_{\infty}^{\infty} V(r) u_1 w_1 dr. \quad (13)$$

The right-hand side is positive since  $V < 0$ , and  $u_1$  and  $w_1$  have equal sign.

The expression (13) is small, since  $V$  is only appreciable in regions where both the functions  $u$  and  $w_1$  are much smaller than outside because of the centrifugal force. For an estimate of (13) we may identify  $u_1$  with

$$w_1 = \frac{\sin kr}{kr} - \cos kr,$$

and obtain

$$\delta_1 = - \frac{M}{\hbar^2 k} \int_{\infty}^{\infty} V(r) (\frac{1}{2} k^2 r^2)^2 dr.$$

From the existence of a small negative eigen-value of the equation (2<sub>0</sub>) one can conclude that

$$-\int V(r) r^4 dr \approx \frac{1}{2} \frac{\hbar^2}{M} a^3$$

$$\delta_1 \approx \frac{1}{18} (ka)^3.$$

Actually the form of  $u_1$  will differ from that of  $w_1$  and therefore the numerical factor will be even less certain; we may write

$$\delta_1 = \frac{\beta}{18} (ka)^3, \quad (14)$$

where  $\beta$  is of order unity. For the special case of a rectangular potential, it may be shown that

$$\beta = \frac{72}{\pi^2} - 6 = 1.32.$$

6. We see that  $\delta_1$  is very small and positive,  $\delta_2, \delta_3$ , etc., are proportional to still higher powers of  $ka$ , and therefore in calculating the deviations from the isotropic distribution we may confine ourselves to the first two terms in (4), and also neglect higher powers of  $\delta_1$  than the first:

$$d\sigma = \frac{\pi}{2k^2} |(\cos 2\delta_0 - 1) + i(\sin 2\delta_0 + 3\delta_1 \cos 0)|^2 \sin \theta d\theta$$

$$= \frac{\pi}{2k^2} (4 \sin^2 \delta_0 + 6\delta_1 \sin 2\delta_0 \cos 0) \sin \theta d\theta.$$

We therefore see that the sign of the asymmetry depends on the product  $\delta_1 \sin 2\delta_0$ . According to the properties of  $\delta_0$  and  $\delta_1$  derived above, we get a maximum backward ( $\cos \theta = -1$ ) for energies smaller than (12), since for these  $\delta_0 > \pi/2$ , i.e.,  $\sin 2\delta_0 < 0$ . At higher energies we have a maximum forward, and the asymmetry vanishes for the energy  $E$ , given by (12).

The highest absolute value of the asymmetry for energies below (12) is obtained for  $E = \frac{1}{2}E_s$ ; then the difference between forward and backward scattering, divided by the average scattering, becomes

$$\beta (\alpha\alpha)^2/12(1-\gamma),$$

which is approximately 1%. Such a small asymmetry is difficult to observe and the anisotropy would become easily observable\* only for neutron energies above (12), i.e., about  $4 \cdot 10^7$  volts, which at the present moment seem impossible to obtain.

It would, however, be very important to measure the angular distribution with neutron energies up to the highest available, in order to ascertain that our original assumptions are at least approximately correct.

If the interaction force is not an "ordinary" one but of the exchange type, the calculation of  $\delta_0$  remains unchanged. In the differential equation for  $\delta_1$ , however, the sign of the potential will be reversed.† To that accuracy with which we considered this potential as a perturbation on  $u$  we simply have to reverse the sign of  $\delta_1$ . Actually also the coefficient  $\beta$  will be smaller than it would be with an "ordinary" force. (With a rectangular potential,  $\beta = \frac{36}{\pi} \frac{1+e^{-r}}{1-e^{-r}} - 6 \left(1 + \frac{12}{\pi^2}\right) = -0.89$ ). Then we shall have a forward maximum for  $E < E_s$ , and a backward maximum for  $E > E_s$ .

#### SUMMARY

The cross-section and the angular distribution are calculated for the scattering of neutrons by protons. The result is practically independent of the special law of force assumed between neutron and proton, it depends only on the known binding energy of the deuteron. The cross-section obtained is about 50% larger than the rather uncertain experi-

\* For energies comparable with  $V$ , i.e., of the order  $10^6$  volts, the asymmetry would become of the order unity.

† Bethe and Peierls, *loc. cit.*

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mental value. The scattering is almost isotropic (in the relative coordinate system) for all neutron energies up to about 40 million volts. Only for still higher energies, which are at present unavailable, an experimental determination of the sign of the anisotropy would decide whether the force between neutron and proton is of the exchange type or an ordinary force.

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## Statistical Theory of Superlattices

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This problem was suggested by W. L. Bragg who, with E. J. Williams, had published a theory of ordered and disordered alloys in analogy with the Weiss theory of ferromagnetism. In the paper, the concept of long- and short-range order is introduced, the latter being higher. It is assumed that only nearest neighbor atoms interact. The statistical problem is treated by an elementary method, it was later done better by Peierls. It is shown that there is a transition temperature at which the long range order disappears. The specific heat associated with the ordering is high just below, low above the transition temperature; there is no latent heat. These are the characteristics of a second phase transition.

## STATISTICAL THEORY OF SUPERLATTICES

By

H. A. Bethe

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## Statistical Theory of Superlattices

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(Communicated by W. L. Bragg, F.R.S.—Received February 13, 1935)

### 1—INTRODUCTION. ANALOGY TO FERROMAGNETISM

In a recent paper, Bragg and Williams\* have pointed out that the arrangement of the atoms in an alloy depends in a striking way on the temperature. At high temperatures, the atoms are distributed practically at random among the lattice points of the crystal, but at low temperatures a superlattice may be formed such that the atoms of one kind are arranged in a regular lattice of their own and the atoms of the other kind occupy the remaining "sites" in the crystal. The transition from the ordered to the disordered state occurs in a fairly small temperature range, and is accompanied by a large specific heat, an increase in electric resistance, etc.

The mathematical method employed by Bragg and Williams is similar to that used in Weiss's theory of *ferromagnetism*. Both involve the assumption that the "force" tending to produce order at a given point is uniquely determined by the average state of order throughout the crystal. Actually it will depend on the configuration of the atoms in the immediate neighbourhood of the point under consideration. The order of the crystal as a whole determines this configuration only on the average. In the present paper, the effect of fluctuations in configuration, which was neglected by Bragg and Williams, will be taken into account.

For our investigation, we shall assume that only nearest neighbours interact. This assumption is essentially the same as that which underlies the modern theory of ferromagnetism.† There we have an interaction energy (electron exchange) between the spins of neighbouring atoms which tries to set them parallel. This interaction, although only acting between neighbouring spins, is nevertheless capable of setting all spins throughout the crystal parallel at low temperatures, thus establishing perfect order. In addition, experimentally a sharp Curie point is found at which the "order," *i.e.*, the permanent moment, of the crystal as a whole dis-

\* 'Proc. Roy. Soc.,' A, vol. 145, p. 699 (1934).

† Bloch, 'Z. Physik,' vol. 61, p. 206 (1930); Bethe, 'Handbuch der Physik,' vol. 24, 2, p. 607.

appears. Super-lattices should be similar, and one may even hope that it is simpler to treat since it involves no quantum mechanics but only classical statistics.

## 2—ORDER AT LARGE AND SMALL DISTANCES. INFLUENCE OF THE NUMBER OF DIMENSIONS

Phenomena analogous to ferromagnetism, such as the one treated in this paper, are essentially restricted to three (or more) dimensions.\* In a linear chain, the interaction between neighbours could never establish order through large distances; there will only be small regions that are ordered. This can be seen very easily for a "linear chain alloy" as follows.

Consider a linear chain containing an equal number of atoms of two different kinds A and B. If there is perfect order, the atoms A and B should simply alternate, giving the arrangement A B A B A B .... At low temperatures, it will indeed be much more probable that two neighbouring atoms should be unlike than like. Still at any finite temperature there will be a finite number of pairs of neighbours of the *same* kind. Consider such a pair, *e.g.*, two neighbouring A-atoms A<sub>1</sub> A<sub>2</sub>. Then the atoms on the right of A<sub>2</sub> will probably be ordered with respect to A<sub>2</sub>, because there is no interaction between them and A<sub>1</sub>. The atoms on the left will be ordered with respect to A<sub>1</sub>, so that the arrangement

$$\dots \text{A B A B}_1 \text{A}_1 \text{A}_2 \text{B}_2 \text{A B A B} \dots$$

arises. The chain falls into two parts which are disordered with respect to each other, *e.g.*, the third atom on the right of B<sub>1</sub> is the B-atom B<sub>2</sub>, whereas in an ordered crystal the third neighbour of a B-atom would be always an A-atom. Thus one single pair of equal neighbours destroys completely the order of the chain as a whole, and only small portions of the chain can be ordered, namely, the portions between any two pairs of like neighbours.

This is completely different for two or three dimensions. Consider in two dimensions again a pair of like neighbours A<sub>1</sub> A<sub>2</sub>. Then it is by no means certain whether a given neighbour of atom A<sub>2</sub>, *e.g.*, the atom x in fig. 1a, is more likely to be a B or an A-atom. For in contrast to the linear chain, x interacts not only with the atom A<sub>2</sub> which would require it to be a B-atom, but also with y, which, being a neighbour of A<sub>1</sub>, should be a B-atom and therefore requires x to be an A-atom. Thus the (prob-

\* Bloc h, *loc. cit.*

able) nature of  $x$  depends on the arrangement of *all* the atoms surrounding it, not only on  $A_2$ . Three alternatives are possible: either

- (1) the atoms surrounding  $A_1 A_2$  "fit" to  $A_1$ , so that  $A_2$  is simply a single "wrong" atom in perfectly ordered surroundings, fig. 1b; or
- (2) the surrounding atoms fit to  $A_2$ , so that  $A_1$  is a "wrong" atom; or
- (3) there is a real break in the order, similar to the linear chain. The crystal falls into two halves, each being completely ordered in itself but completely disordered with respect to the other half. The halves are separated from each other by a "boundary" which passes between  $A_1$  and  $A_2$  and also between other pairs of neighbouring like atoms, fig. 1c.

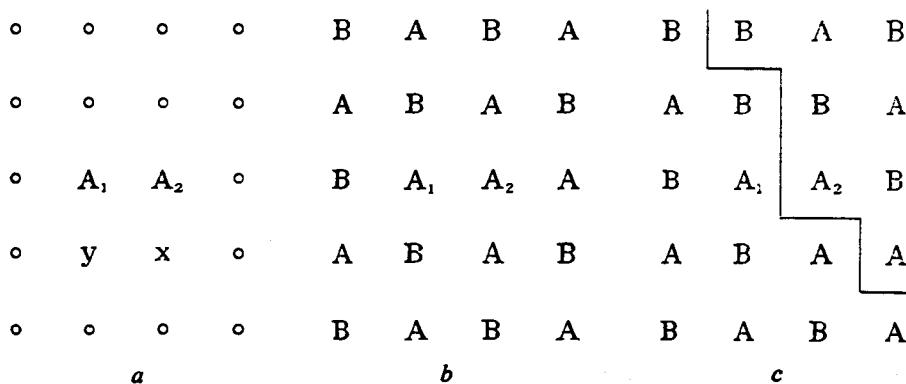


FIG. 1

It is clear at once that—given the existence of the pair  $A_1 A_2$ —the arrangements (1) and (2) have lower energy than (3). For in the first two cases we need only have four pairs of like neighbours, e.g., in case (1)  $A_2$  is surrounded by 4 A-atoms whereas everywhere else we have only pairs of unlike neighbours. In case (3), on the other hand, we have one pair of equal neighbours *per unit length of the boundary*, and this makes an enormous number of pairs if we want the boundary to extend through the whole crystal, thus really destroying the correlation between left-hand side and right-hand side of the crystal, in analogy to the linear chain.

At low temperatures, only the states of low energy are realized, therefore we expect that at low temperatures the crystal is ordered as a whole, only containing the few atoms at wrong places inside it, e.g., a cubic body-centred crystal would have nearly all corners of the cubes occupied

by A-atoms and almost all centres by B-atoms; only a small fraction of the A-atoms (increasing with temperature) goes into the centres and a corresponding number of B-atoms occupies corners.\*

We have at low temperatures a "correlation" between distant atoms, however far away. If we know the nature of the atom situated at a given place, we can predict whether another atom 1000 atomic distances away is likely to be an A- or a B-atom.

This will not be true for high temperatures. For then the number of possible realizations of a given arrangement of atoms is more important than the energy of the arrangement. Given only the two atoms  $A_1$  and  $A_2$ , there is only one single arrangement of the atoms in the crystal corresponding to case (1) above, since the positions of all atoms are fixed by requiring that there should be perfect order with respect to  $A_1$ . But there is an immense number of ways in which a boundary may be laid through the crystal; therefore, at sufficiently high temperatures, case (3) is the more probable *in spite of its higher energy*. Thus the "correlation of distant atoms" disappears at high temperatures (§ 6).

This does not mean that there is no order at all at high temperatures. At any finite temperature, it will be more likely to find a B-atom beside a given A-atom than to find another A-atom there, because the energy is smaller in the former case and the *a priori* probability is the same. Only the order does not extend through the whole (and not even through large portions of the) crystal. Thus we are led to distinguish between two different types of order: the order of neighbours and the order of the crystal as a whole (order at large distances).

### 3—DEFINITION OF THE TWO DEGREES OF ORDER

The "order of neighbours"  $\sigma$  is defined as the difference of the probabilities of finding an unequal and an equal neighbour beside a given atom. Thus the probability for finding a B-atom beside a given A-atom is  $\frac{1}{2}(1 + \sigma)$ , that for finding another A-atom is  $\frac{1}{2}(1 - \sigma)$ . If  $N$  is the total number of atoms,  $z$  the number of neighbours of each atom, then there will be

$$\begin{aligned} \frac{1}{4}Nz(1 + \sigma) &\text{ pairs of neighbours A B,} \\ \frac{1}{4}Nz(1 - \sigma) &\text{ pairs A A and equally many B B.} \end{aligned}$$

If the interaction energy between an A and a B atom is  $V_{ab}$ , and  $V_{aa}$  and

\* Of course, the B-corners and A-centres in the equilibrium state will *not* in general be beside each other.

$V_{bb}$  that between A A and B B respectively, the total energy of our crystal becomes

$$E = \frac{1}{4}NzV_{ab}(1 + \sigma) + \frac{1}{8}Nz(V_{aa} + V_{bb})(1 - \sigma) = \text{const} + \frac{1}{4}NzV(1 - \sigma), \quad (1)$$

where

$$V = \frac{1}{2}(V_{aa} + V_{bb}) - V_{ab}. \quad (2)$$

Thus the order of neighbours  $\sigma$  is directly proportional to the energy of the crystal (apart from a constant).  $V$  is the difference of the interaction energies between two equal and between two unequal neighbours.  $V$  must be positive in order to make a superlattice possible (otherwise the atoms A and B would segregate). Its magnitude determines the temperature at which the transition from the ordered to the disordered state takes place.  $\sigma = 1$  corresponds to perfect order,  $\sigma = 0$  to perfect disorder. For any finite temperature  $\sigma$  lies between these limits.

To define the long-distance order, we divide the lattice points in the crystal into two groups,  $a$  and  $b$ , the points of each group forming a lattice of their own, e.g., in a cubic body-centred lattice,  $a$  and  $b$  are the corners and the centres of the cubes; in a simple cubic lattice the  $a$ 's and  $b$ 's form a rocksalt structure, the positions of the Na atoms being denoted as "a," the Cl positions as "b." Then the long-distance order  $S$  is the probability for finding an A-atom in an "a" position minus the probability for finding a B-atom there. This definition of order is equivalent to that used by Bragg and Williams.  $S = +1$  or  $-1$  corresponds to perfect order,  $S = 0$  to perfect disorder. Above a certain critical temperature  $\Theta$  (Curie point) we expect  $S$  to be zero (§ 2), below  $\Theta$  the "distant order"  $S$  is finite.

If  $S$  is to have a physical meaning, it is necessary that the temperature at which the distant order disappears should be independent of the size of the crystal; in other words that the question of stability or non-stability of breaks in the order should not depend on the number of atoms in the crystal but only on the temperature. This can be proved for two- and three-dimensional lattices.\*

#### 4—QUALITATIVE DISCUSSION OF THE TRANSITION POINT

For a given value of  $S$ , there is a great number of possible distributions of the atoms over the various sites. We know only that there are

\* The probability for a boundary is of the order  $\exp\left(e^{\frac{NV}{k}\left(\frac{1}{T} - \frac{1}{T_0}\right)}\right)$ ,  $N$  being the number of atoms in one crystal plane,  $T_0$  a critical temperature and  $k$  Boltzmann's constant.

$\frac{1}{4}N(1 + S)$  A-atoms and  $\frac{1}{4}N(1 - S)$  B-atoms in *a*-positions. But they may be distributed over the  $\frac{1}{2}N$  available *a*-positions in  $\binom{\frac{1}{2}N}{\frac{1}{4}N(1 - S)}$  different ways, and there is an equal number of possible distributions of A- and B-atoms over the *b*-positions. Each distribution corresponds to a certain energy. The lowest energy is obtained if all "wrong" atoms, *i.e.*, the B-atoms in *a*-positions and the A-atoms in *b*-positions, are put together. They then form a cluster inside which there is perfect order, and only on the surface are there then pairs of like neighbours. The energy is only of the order  $N^{2/3}(1 - S)^{2/3}V$  if the constant in 1 is put equal to zero. It is, however, clear that this distribution is most unlikely, and that it is much more probable that the "wrong" atoms are more or less isolated from each other. For complete isolation, we obtain the maximum possible energy, *viz.*,  $\frac{1}{2}NzV(1 - S)$ . There is a great number of states having energies between these two limits.

We may suppose the number of states having a given *S* and a given energy (or  $\sigma$ ) to be given; let us denote this number by  $n(S\sigma)$ . Then we can calculate the partition function for any value of *S* at a given temperature *T*

$$P(S) = \sum_{\sigma} n(S\sigma) e^{-E(\sigma)/kT}.$$

By symmetry we have  $P(-S) = P(S)$ . At very low temperatures the partition function will have two maxima at  $S = \pm 1$  and a minimum at  $S = 0$ . As the temperature increases, the maxima move to lower (absolute) values of *S*, *i.e.*, the long-distance order decreases gradually. This goes on until the two maxima merge into each other at  $S = 0$ , at a certain critical temperature  $\Theta$ .\*

The energy of the crystal increases with temperature for two reasons: Firstly, for a given *S* the average energy increases ( $\sigma$  decreases) with temperature. In other words, if *S* is kept fixed, the "wrong atoms" cluster together at low temperatures and become isolated at high temperatures. The specific heat due to this process (*i.e.*, the rate of change of the energy with temperature) almost certainly decreases with increasing temperature for any given value of *S*.

\* These statements cannot be proved rigorously, but seem highly probable. An alternative assumption would be that a secondary maximum develops at  $S = 0$ , increases gradually with increasing temperature and becomes higher than the two maxima at large *S*, before the latter have merged together. In this case, there would be a real point of transformation, with latent heat, jump in the physical properties, etc. But there seems to be neither a theoretical nor an experimental reason for such an assumption.

Secondly, the most probable large-distance order decreases with increasing temperature until it reaches zero at  $T = \Theta$ . Since for small  $S$  there are many states with rather high average energy, for large  $S$  few states with low energy, the change of  $S$  means also an increase of energy. The corresponding specific heat should increase with increasing temperature, since the long-distance order changes (decreases) the more rapidly the smaller it is already, *i.e.*, the nearer the temperature comes to  $\Theta$  (*see* Bragg and Williams, *loc. cit.*, and § 6 of this paper). When the critical temperature  $\Theta$  is reached, this second kind of specific heat suddenly disappears altogether. Therefore we should expect (1) a jump in the specific heat at  $T = \Theta$ , *i.e.*, a higher  $c_v$  for  $T < \Theta$  than for  $T > \Theta$ , (2) the specific heat should increase with increasing temperature on the low-temperature side of the critical temperature, since it contains the specific heat due to change of long-distance order on that side, (3) it should decrease on the high-temperature side, because there it is entirely due to the change of average energy for the fixed value  $S = 0$ .

All these features are shown by the curves  $d$  and  $e$  in fig. 6, which give the results of the quantitative calculation. The contribution from the disordering to the specific heat above the "Curie point" is seen to be exceedingly small, only about 5% of that below  $\Theta$ . The theory of Bragg and Williams gives zero specific heat above  $\Theta$ , because it considers only the specific heat due to change of  $S$ .

All physical properties which depend on the order at long distances, such as electric conductivity, and more so the intensity of the super-lattice lines in X-ray spectra, should show a rapid change below  $T = \Theta$ , and have practically the value for a perfectly disordered crystal above  $\Theta$ . There should be no jump in these quantities at  $T = \Theta$ , but only a kink in the curves representing them as functions of  $T$ .

### 5—APPROXIMATION FOR VANISHING LONG-DISTANCE ORDER

At high temperature there is no order at long distances. There is, however, a considerable correlation between neighbours which we shall calculate.

Let  $w = \frac{1}{2}(1 - \sigma)$  be the probability that a neighbour of a given "central" A-atom is itself an A-atom. For a first approximation, we could assume this probability to be independent of the nature of the other neighbours of the central atom. Then obviously the ratio of the probabilities that the neighbour is A or B respectively is given by the Boltzmann factor

$$e^{-V/kT} = x, \quad (3)$$

viz.,

$$w/(1 - w) = x,$$

from which we find

$$\sigma = (1 - x)/(1 + x). \quad (4)$$

This means a very slow increase of the order with decreasing temperature (decreasing  $x$ ) which is shown in fig. 4, curve *a*. There is no sign whatever of a "transition temperature."

The assumed mutual independence of the neighbours of one central atom is, however, only true for a linear chain of atoms. For two- or three-dimensional lattices, the nearest neighbours of a central atom ("atoms in the first shell") are connected with each other not only by their interaction with the central atom but also by interaction with the "second shell" which is defined as containing all the nearest neighbours

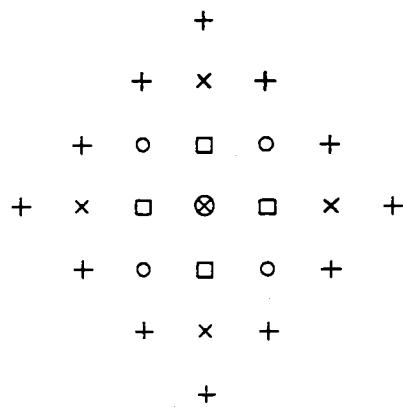


FIG. 2—Quadratic lattice.  $\otimes$  Central atom;  $\square$  first shell;  $\times$  corner atoms in second shell;  $\circ$  medium atoms, second shell;  $+$  third shell

of the atoms in the first shell, fig. 2. This interaction tends to make all atoms in the first shell equal, and thus supports the ordering force exerted by the central atom. Therefore the order is greater than in our first approximation for any temperature and the order-temperature curve is steeper.

The effect of the second shell can be taken into account by the following method (second approximation). Take a given distribution of A- and B-atoms over the first shell and calculate the partition function for this distribution, including the interaction with the second shell. We shall explain this for the quadratic (two-dimensional) lattice, fig. 2. Each lattice point has, in this system, four nearest neighbours, this is therefore the number of atoms in the first shell. The second shell contains 8 atoms, 4 of which lie at the corners of a square and 4 at the middle of its sides ("medium atoms"). The following distributions are possible.

(1) *No A-atoms in the First Shell*—Then the interaction energy of the first shell with the central atom is zero.\* If any corner-atom in the second shell is A, its interaction energy with its neighbour in the first shell (which is certainly a B-atom) is zero as well. If the corner-atom is B, the interaction energy is V. Therefore, each corner-atom has the partition function (p.f.).

$$1 + e^{-V/kT} = 1 + x.$$

If a medium position of the second shell is occupied by an A-atom, the latter's interaction energy with the first shell is again zero, while a B-atom would have the interaction energy  $2V$ , because it interacts with two B-atoms in the first shell. Therefore its p.f. becomes

$$1 + e^{-2V/kT} = 1 + x^2.$$

Each atom in the second shell can, in our approximation, be treated separately; therefore the total p.f. is simply the product of the p.f.'s for the single atoms in the second shell, viz.,

$$P_0 = (1 + x^2)^4 (1 + x)^4.$$

The index 0 signifies that there is no A-atom in the first shell.

(2) *One A-atom in the First Shell*—The interaction energy with the central atom is now 1 (we leave the factor  $V$  out), giving a factor  $x$  in the p.f. Furthermore, there are four possible positions for the A-atom in the first shell, so we have a statistical weight 4. For the corner-atoms in the second shell, the p.f. is not changed, e.g., for the corner near the A-atom of the first shell, the energy is now 0 if the corner is occupied by a B-atom and 1 if the atom is A, but the p.f. remains  $1 + x$ . For the medium atoms, however, two positions are to be distinguished: two medium atoms, marked  $\circ$  in fig. 3a, have still got two B-atoms as neighbours and have thus the p.f.  $1 + x^2$ . The two others, marked  $\times$ , each have one A and one B neighbour; it is therefore irrelevant whether they are A or B, in any case their interaction energy with their neighbours in the first shell will be 1, which makes the p.f. for them  $2x$ . Therefore the total partition function is

$$P_1 = 4x(2x)^2(1 + x^2)^2(1 + x)^4.$$

(3) *Two Atoms in the First Shell*—They can lie (a) side by side, para-position, fig. 3b, or (b) opposite each other, ortho-position, fig. 3c. The

\* We fix the interaction energy of two unequal neighbours to be zero, that of two equal neighbours has then to be taken equal to  $V$  (cf. equation (2)). The constant in (1) is then zero.

interaction with the central atom is 2 in both cases, giving factor  $x^2$ . The statistical weight for para 4, for ortho 2. Partition function for each corner atom  $1 + x$ . Medium atoms of second shell:

(a) for para two medium atoms have two like neighbours (one A A the other B B) and therefore p.f. =  $1 + x^2$ , the other two have neighbours A B, p.f. =  $2x$ . Consequently,

$$P_{2P} = 4x^2(2x)^2(1+x^2)^2(1+x)^4;$$

(b) for ortho each medium atom has one A- and one B-neighbour, giving  $2x$  for its p.f., therefore

$$P_{2O} = 2x^2(2x)^4(1+x)^4.$$

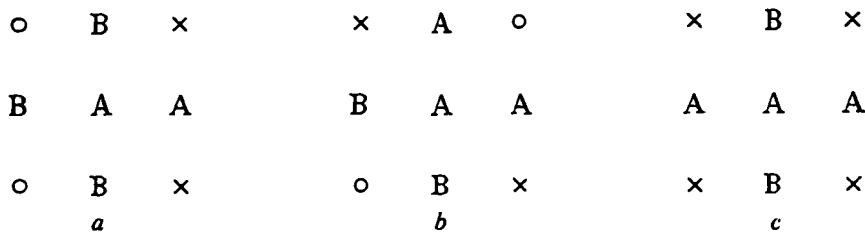


FIG. 3

(4) For three A-atoms the interaction with the second shell is the same as for one A in the first shell, the interaction with the central atom is 3 instead of 1, giving

$$P_3 = 4x^3(2x)^2(1+x^2)^2(1+x)^4.$$

(5) Four A-atoms are identical with no one as regards interaction with the outside, the interaction with the centre is 4 instead of 0, therefore

$$P_4 = x^4(1+x^2)^4(1+x)^4.$$

The probability that a "central" A-atom has no A-atom among its neighbours is now

$$p_0 = P_0/(P_0 + P_1 + P_{2P} + P_{2O} + P_3 + P_4).$$

The average number of A-atoms near a central A-atom is

$$w = \frac{P_1 + 2(P_{2P} + P_{2O}) + 3P_3 + 4P_4}{P_0 + P_1 + P_{2P} + P_{2O} + P_3 + P_4} = p_1 + 2(p_{2P} + p_{2O}) + 3p_3 + 4p_4,$$

and the degree of order

$$\sigma = 1 - \frac{1}{2}w = p_0 - p_4 + \frac{1}{2}(p_1 - p_3). \quad (5)$$

The order calculated by this method is considerably larger than in the first approximation (formula (4)), and increases with temperature more steeply. For the quadratic lattice we have

$x =$	0·1	0·2	0·3	0·4	0·5	0·6	0·8	1·0
(first approx.) ..	81·8	66·7	53·8	42·9	33·3	25·0	11·1	0
(second approx.)	99·03	91·71	75·6	56·6	40·4	28·2	11·9	0

For the simple cubic lattice the order is given in fig. 4 (curve *b*) as a function of temperature.

It would in principle be possible to reach the exact value for the order at any temperature by calculating the higher approximations of our method. Actually, already the third approximation is extremely tedious, so that a more direct method is required which considers long-distance order.

The effect of our second approximation as compared with the first is to make it improbable that two neighbouring atoms in the first shell are unequal.\* If we divide all the partition functions  $P_0 P_1 P_2 \dots$  by  $P_0$ , we get simply

$$P_{mn} = g_{mn} x^n \left( \frac{2x}{1+x^2} \right)^m \quad (6)$$

where  $n$  is the number of A-atoms in the first shell,  $g_{mn}$  the statistical weight and  $m$  the number of pairs of unequal neighbours in the first shell, *i.e.*, for each such pair the partition function has to be multiplied by the factor

$$\mu = \frac{2x}{1+x^2} \quad (7)$$

which takes account of the interaction with the second shell.

#### 6—FIRST APPROXIMATION INCLUDING LONG-DISTANCE ORDER

With the notation of § 3, we may divide the atoms into “right” ones, (R-atoms) and wrong ones (W-atoms). An A-atom in an “*a*” position or a B-atom in a “*b*” position are “right,” and A-atom in “*b*” or a B-atom in “*a*” are to be termed W. Two neighbouring R-atoms or two neighbouring W-atoms have the interaction energy zero; a pair of neighbours R W has the interaction energy  $V$ .

\* Two neighbours in a given shell are, of course, never nearest neighbours but only second nearest. The nearest neighbours of an atom in the  $n$ th shell lie all in the  $n - 1$ st and  $n + 1$ st shells. Nearest neighbours have to be unlike, second nearest like if the crystal is perfectly ordered. The number of pairs of *unequal neighbours in a given shell* is therefore the smaller the greater the order.

We consider again a central atom and the various shells round it (§ 5). In the first approximation, we assume that the only effect of the "outer shells" is to make R-atoms in the first shell more likely than W-atoms. This is due to the fact that the outer shells themselves contain more R-atoms than W's, according to our assumption, and that the energy is smaller if an R-atom lies beside another R than if a W-atom lies there. To take account of this fact we introduce a factor  $\epsilon$  into the partition function for each wrong atom in the first shell. We can then calculate the probabilities (a) that the central atom is wrong, (b) that any atom in the first shell is wrong, as functions of  $x$  (temperature) and  $\epsilon$ . The parameter  $\epsilon$  is then fixed by the condition that the two probabilities (a) and (b) must be equal, because the "central" atom is in no way distinguished from the others.

Let us suppose that each atom in the crystal has  $z$  nearest neighbours. Then the partition function (relative probability), that the central atom is R and  $n$  of the atoms in the first shell are wrong, is

$$r_n = \binom{z}{n} x^n \epsilon^n. \quad (8)$$

Here  $\binom{z}{n}$  is the statistical weight (number of distributions of the  $n$  wrong atoms over the  $z$  sites), one factor  $x$  is introduced for the interaction of the central R-atom with any one W-atom in the first shell, and  $\epsilon^n$  takes account of the interaction with the outside. If the central atom is wrong, its interaction energy with the first shell is  $(z - n)V$ , because it has the interaction energy  $V$  with each R-atom. Therefore the probability that the centre is W and  $n$  wrong atoms are in the first shell, becomes

$$w_n = \binom{z}{n} x^{z-n} \epsilon^n. \quad (8A)$$

Accordingly, the total relative probabilities that the central atom is right or wrong are respectively

$$\left. \begin{aligned} r &= \sum_{n=0}^z r_n = (1 + \epsilon x)^z \\ w &= \sum w_n = (\epsilon + x)^z \end{aligned} \right\}. \quad (9)$$

On the other hand, the relative probability that an atom of the first shell is wrong is given by

$$w' = \frac{1}{z} \sum n(r_n + w_n) = \frac{1}{z} \epsilon \frac{\partial}{\partial \epsilon} (r + w) = \frac{\epsilon x}{1 + \epsilon x} r + \frac{\epsilon}{\epsilon + x} w. \quad (10)$$

The condition

$$w' = w \quad (11)$$

therefore reduces to

$$\left. \begin{aligned} \frac{x}{\varepsilon + x} w &= \frac{\varepsilon x}{1 + \varepsilon x} r \\ \frac{w}{r} &= \frac{\varepsilon(\varepsilon + x)}{1 + \varepsilon x} \end{aligned} \right\}, \quad (12)$$

whereas from (9) we find

$$\frac{w}{r} = \left( \frac{\varepsilon + x}{1 + \varepsilon x} \right)^z. \quad (13)$$

Comparing (12) and (13), we obtain

$$(\varepsilon + x)/(1 + \varepsilon x) = \varepsilon^{1/(z-1)}, \quad (13A)$$

therefore

$$x = (\varepsilon^{1/(z-1)} - \varepsilon)/(1 - \varepsilon^{z/(z-1)}),$$

and, putting

$$\varepsilon = e^{-2\delta(z-1)}, \quad (13B)$$

we have

$$x = \sinh(z-2)\delta/\sinh z\delta. \quad (14)$$

From this equation,  $\varepsilon$  may be determined as a function of the temperature, *i.e.*, of  $x$ , or more easily  $x$  as function of  $\varepsilon$ . One sees immediately:

(1) Two values of  $\varepsilon$ , namely,  $\varepsilon = \varepsilon'$  and  $\varepsilon = 1/\varepsilon'$ , correspond to the same value of  $x$ . That means that "right" and "wrong" atoms may be interchanged, as is natural.

(2) The value  $\varepsilon = 1$  always gives a solution, namely,  $x = 0/0$ . This is to be understood from the fact that the case  $S = 0$ , *i.e.*, no long-distance order, always corresponds to an extreme of the free energy, namely, a minimum at high, a maximum at low temperature.

(3) If  $\varepsilon$  is different from unity,  $x$  can never be larger than

$$x_0 = 1 - 2/z. \quad (15)$$

For (14) evidently increases with increasing  $\varepsilon$  (decreasing  $\delta$ ) as long as  $\delta > 0$ . The maximum value of (14) is therefore obtained by putting  $\delta \ll 1$ ; this leads to the value (15) for  $x$ .

Order at large distances can therefore only exist below a critical temperature, which is given by (15). Above that temperature, (14) has only the one solution  $\varepsilon = 1$ , corresponding to  $S = 0$ . Below  $\Theta$ , there are three solutions,  $\varepsilon'$ , 1,  $1/\varepsilon'$ , the first and third of which correspond to a non-vanishing order  $+S$  and  $-S$  at long distances and to a lower free energy than  $\varepsilon = 1$ .

The energy of the crystal is  $V$  times the number of pairs of neighbours  $RW$ . This number is equal to the total number of atoms  $N$ , times the

probability for right atoms,  $r/(w+r)$ , times the average number of wrong neighbours of a right atom,  $\Sigma(nr_n)/r$ . Therefore

$$E = NV\Sigma(nr_n)/(w+r).$$

Using (1), we can calculate the order of neighbours

$$1 - \sigma = \frac{4}{z} \frac{\Sigma nr_n}{w+r}, \quad (16)$$

which according to (9), (10) becomes

$$1 - \sigma = 4 \frac{\varepsilon x}{1 + \varepsilon x} \frac{r}{w+r}. \quad (17)$$

Now from (13) and (13A) we deduce (*cf.* 13B)

$$w/r = \varepsilon^{z/(z-1)} = e^{-2z\delta}, \quad (18)$$

so that

$$1 - \sigma = 4 \frac{\varepsilon x}{1 + \varepsilon x} \frac{1}{1 + \varepsilon^{z/(z-1)}} = \frac{2 \sinh(z-2)\delta}{\sinh(2z-2)\delta \cosh z \delta} \quad (19)$$

where  $\varepsilon$  may be expressed in terms of  $x$ , by making use of (14).

The order at long distances is simply

$$S = \frac{r-w}{r+w} = \tanh z\delta. \quad (20)$$

This reaches zero at the critical temperature ( $\varepsilon = 1$ ), whereas for the order of neighbours at that temperature we find (*cf.* (17), (15))

$$1 - \sigma_0 = 2 \frac{x_0}{1+x_0}; \quad \sigma_0 = \frac{1-x_0}{1+x_0} = \frac{1}{z-1}. \quad (21)$$

We now proceed to calculate the specific heat near the critical temperature. We find from (14), (20)

$$x = \frac{z-2}{z}(1 - \frac{2}{3}(z-1)\delta^2 + \dots), \quad (14A)$$

$$S = z\delta - \dots, \quad (20A)$$

and, after some calculation,

$$1 - \sigma = \frac{z-2}{z-1}(1 - \delta^2 z(z-\frac{2}{3}) + \dots), \quad (19A)$$

$$\frac{d(1-\sigma)}{dx} = \left(\frac{z}{z-1}\right)^2 (\frac{5}{2}z-1). \quad (22)$$

For the specific heat per atom we obtain, using (1) and (3)

$$\left. \begin{aligned} c_v &= \frac{dE}{N dT} = \frac{z}{4} kx (\log x)^2 \frac{d(1-\sigma)}{dx} \\ &= \frac{z-2}{4} \left( \frac{z}{z-1} \right)^2 \left( \frac{3}{2}z - 1 \right) \left( \log \frac{z-2}{z} \right)^2 k \end{aligned} \right\}. \quad (23)$$

Above the critical temperature, we have according to (4),

$$\sigma = (1-x)/(1+x),$$

therefore

$$\left( \frac{d(1-\sigma)}{dx} \right)_{x>\infty} = \frac{2}{(1+x_0)^2} = \frac{1}{2} \left( \frac{z}{z-1} \right)^2, \quad (24)$$

and the ratio of the specific heat below and above  $\Theta$  becomes

$$\frac{c_v(T < \Theta)}{c_v(T > \Theta)} = 3z - 2. \quad (25)$$

Numerically, we obtain the following values for the specific heat just above and below the Curie point:—

Number of neighbours	Structure	Specific heat per atom	
		Below	Above
2	linear chain	0	0
4	quadratic	2.14 k	0.214 k
6	simple cubic	1.90	0.119
8	cubic body-centred	1.78	0.081
12	cubic face-centred	1.68	0.049
$\infty$	—	1.50	0

The long-distance order changes near the Curie point as the root of  $\Theta - T$ , viz., according to (14A) and (20A),

$$\begin{aligned} S &= z\delta = z \sqrt{\frac{3}{2(z-1)}} \sqrt{\frac{x_0-x}{x_0}} = z \sqrt{\frac{3|\log x_0|}{2(z-1)}} \sqrt{\frac{\Theta-T}{\Theta}} \\ &= \sqrt{\frac{3}{2} \frac{z^2}{z-1} \log \frac{z}{z-2}} \sqrt{\frac{\Theta-T}{\Theta}}, \end{aligned} \quad (26)$$

e.g., for a simple cubic lattice  $S = 2.09 \sqrt{(\Theta-T)/\Theta}$ , for  $z = \infty$ , we have  $S = 1.73 \sqrt{(\Theta-T)/\Theta}$ . The long-distance order increases the more rapidly with decreasing temperature the smaller the number of neighbours of each atom. Accordingly, the specific heat near the Curie point also increases with decreasing  $z$ .

## 7—COMPARISON WITH THE THEORY OF BRAGG AND WILLIAMS

For an infinite number of neighbours  $z$ , our theory goes over exactly into that of Bragg and Williams, putting their  $V_0$  equal to  $2z$  times our  $V$ .

If we introduce  $\delta$  as in (13B),  $z\delta$  must be of order unity because of (20A), therefore  $\delta \ll 1$ , and according to (14A), (20)

$$x = \frac{\sinh(z-2)\delta}{\sinh z\delta} = 1 - \frac{2\delta}{\tanh z\delta} = 1 - \frac{2\delta}{S}.$$

On the other hand,  $V/kT$  is small in the interesting temperature range, since  $zV/kT$  is of the order unity. Therefore the definition (3) for  $x$  becomes

$$x = 1 - V/kT = 1 - 2\delta/S,$$

which means

$$\delta = VS/2kT.$$

Introducing this into (20A), we find

$$S = \tanh z\delta = \tanh(VzS/2kT) = \tanh(V_0S/4kT),$$

i.e., the principal equation of the theory of Bragg and Williams.

For the "order of neighbours" follows from (19)

$$1 - \sigma = 4 \frac{1}{(\cosh z\delta)^2}; \quad \sigma = (\tanh z\delta)^2 = S^2,$$

also identical with the assumption of Bragg and Williams. Therefore all consequences of their theory also follow from our first approximation for  $z = \infty$ .

## 8—SECOND APPROXIMATION

The "outer shells" have not only the effect of making the atoms in the first shell "right"—which we treated in § 6—but also of making them equal to each other, as we know from § 5. We now make essentially the same approximation as in § 5, only we assume in addition that the outer shells make it more probable to find an R-atom in the second shell than a W-atom. We therefore introduce, as in § 6, a factor  $\epsilon$  in the partition function for each wrong atom in the second shell, and we determine  $\epsilon$  from the condition that the probability to find a wrong atom is the same for the centre atom as for an atom in the first shell.

The reasoning is now exactly similar to § 5. Consider, e.g., a corner atom in the second shell beside a right atom in the first. The contribution to the partition function is simply unity, if the corner atom is right, and it is  $\epsilon x$  if the atom is "wrong," where the factor  $x$  arises from

the interaction with the neighbour in the first shell (as in § 5), while  $\epsilon$  is introduced by the interaction with the outer shells. Thus the p.f. of the corner atom is  $1 + \epsilon x$  if it lies beside an R-atom in the first shell, and similarly it may be shown to be  $x + \epsilon$  if the neighbouring first shell atom is W.

The factor in the p.f. corresponding to a "medium atom" in the second shell is

- $1 + \epsilon x^2$ , if its two nearest neighbours in the first shell are both R;
- $\epsilon + x^2$ , if both nearest neighbours are W;
- $x(1 + \epsilon)$ , if one of them is a W, the other an R-atom.

For  $\epsilon = 1$  these formulæ go over into those of § 5.

A given configuration of the first shell may be characterized by the number  $n$  of wrong atoms in the shell and the number  $m$  of pairs of unequal neighbours in it.\* Then the number of R-atoms is  $z - n$ , the number of neighbouring pairs WW is  $(\frac{1}{2}z - 1)n - \frac{1}{2}m$ , and the number of pairs RR is  $(\frac{1}{2}z - 1)(z - n) - \frac{1}{2}m$ . For each atom in the first shell of a quadratic or simple cubic lattice has  $z - 2$  neighbours in the first shell, viz., all atoms of that shell except the diametrically opposite and itself. Therefore we have

$$(z - 2) \times \text{number of W-atoms} = \text{number of RW-pairs} + 2 \times \text{number of WW-pairs},$$

$$(z - 2) \times \text{number of R-atoms} = \text{number of RW-pairs} + 2 \times \text{number of RR-pairs},$$

which gives the above expressions for the number of RR and WW pairs.

If we now put equal to unity, the partition function that *all* atoms of the first shell are R, we have to introduce a factor  $(\epsilon + x)/(1 + \epsilon x)$  for each W-atom in the first shell (because of the interaction with corner atoms), a factor  $(\epsilon + x^2)/(1 + \epsilon x^2)$  for each pair of neighbours WW, and a factor  $x(1 + \epsilon)/(1 + \epsilon x^2)$  for each pair RW.

Therefore the partition function for any configuration of the first shell becomes

$$P_{nm} = g_{nm} \left( \frac{\epsilon + x}{1 + \epsilon x} \right)^n \left( \frac{\epsilon + x^2}{1 + \epsilon x^2} \right)^{(\frac{1}{2}z-1)n - \frac{1}{2}m} \left( \frac{x(1 + \epsilon)}{1 + \epsilon x^2} \right)^m \quad (27)$$

with  $\lambda = \frac{\epsilon + x}{1 + \epsilon x} \left( \frac{\epsilon + x^2}{1 + \epsilon x^2} \right)^{\frac{1}{2}z-1} \quad (28)$

$$\mu = \frac{x^2(1 + \epsilon)^2}{(1 + \epsilon x^2)(\epsilon + x^2)}$$

\* Cf. footnote, p. 556.

$g_{nm}$  = statistical weight. It is more convenient to divide (27) by  $\lambda^z$ , so that

$$P'_{nm} = g_{nm} \lambda^{n-\frac{1}{2}z} \mu^{\frac{1}{2}m}. \quad (27A)$$

It remains to consider the interaction with the central atom. The partition function that the central atom is right and that  $n$  wrong atoms occur in the first shell, becomes

$$r_{nm} = P'_{nm} x^n, \quad (29)$$

and the partition function of the same configuration with a wrong central atom is

$$w_{nm} = P'_{nm} x^{z-n}. \quad (29A)$$

The parameter  $\epsilon$  has to be fixed by the condition of equal "long-distance order" at the centre and in the first shell:

$$\sum_{nm} w_{nm} = \frac{1}{Z} \sum_{nm} n (r_{nm} + w_{nm}), \quad (30)$$

the order of neighbours is then given by (16).

In discussing these equations, we first consider the "Curie point." Near that point,  $\epsilon$  may be put equal to  $1 - \delta$  with  $\delta \ll 1$ . Then

$$\lambda = 1 - \delta \left[ \frac{1-x}{1+x} + (\frac{1}{2}z-1) \frac{1-x^2}{1+x^2} \right] + \dots,$$

whereas

$$\mu = \left( \frac{2x}{1+x^2} \right)^2 \left[ 1 + \frac{1}{4}\delta^2 \left( \frac{1-x^2}{1+x^2} \right)^2 + \dots \right].$$

Therefore, neglecting  $\delta^2$ , we have

$$\begin{aligned} \mu &= \mu_0 = (2x/1+x^2)^2, \\ \lambda &= 1 - \kappa, \quad \kappa \ll \delta \ll 1. \end{aligned} \quad \} \quad (31)$$

Then

$$r_{nm} = g_{nm} x^n \mu_0^{\frac{1}{2}m} (1 - (n - \frac{1}{2}z) \kappa) = p_{nm} (1 + (\frac{1}{2}z - n) \kappa), \quad (32)$$

where  $p_{nm}$  is the probability for the configuration  $nm$  as calculated in § 5, i.e., assuming no long-distance order. It is simply a function of  $x$  (temperature), and  $\epsilon$  enters the probability  $r_{nm}$  only in the factor

$$1 + (\frac{1}{2}z - n) \kappa.$$

Adding the probabilities of the various configurations having the same number  $n$  of W-atoms in the first shell, we may rewrite (32):

$$r_n = p_n (1 + (\frac{1}{2}z - n) \kappa), \quad (32A)$$

$p_n$  is the probability that—with no long-distance order— $n$  atoms of the first shell are *equal* to the central atom.

Similarly, we obtain

$$w_n = p_{z-n} (1 + (\frac{1}{2}z - n) \kappa) \quad (32B)$$

because, if the central atom is wrong, all the *right* atoms of the first shell are equal to it, *i.e.*,  $z - n$  atoms. Summing (32A) over  $n$ , we obtain

$$r = \sum p_n + \sum (\frac{1}{2}z - n) p_n \kappa = 1 + \frac{1}{2}z\kappa\sigma_0. \quad (33)$$

For  $\sum p_n$  is the sum of the probabilities of all configurations of the first shell and therefore unity, whereas

$$\sum \left(1 - \frac{2n}{z}\right) p_n = \sigma_0 \quad (34)$$

is the probability of finding (with vanishing long-distance order) an unequal atom beside the central atom minus that of finding an equal one there ( $z - n$  of the  $z$  first shell atoms are unequal,  $n$  equal to the central atom).

Similarly to (33), we obtain

$$w = \sum w_{z-n} = \sum p_n (1 - (\frac{1}{2}z - n) \kappa) = 1 - \frac{1}{2}z\kappa\sigma_0, \quad (33A)$$

$$\frac{2}{z} \sum n r_n = r - \sum \left(1 - \frac{2n}{z}\right) r_n = r - \sigma_0 - \frac{1}{2}z\kappa\sigma_0, \quad (35)$$

$$\begin{aligned} \frac{2}{z} \sum n w_n &= \frac{2}{z} \sum (z - n) w_{z-n} = w + \sum \left(1 - \frac{2n}{z}\right) w_{z-n} \\ &= w + \sigma_0 - \frac{1}{2}z\kappa\sigma_0, \end{aligned} \quad (35A)$$

where

$$\rho = \sum \left(1 - \frac{2n}{z}\right)^2 p_n. \quad (36)$$

Adding (35) and (35A) and using (30), we obtain

$$\left. \begin{aligned} 2w &= \frac{2}{z} \sum n (r_n + w_n) = r + w - z\kappa\sigma_0 \\ r - w &= z\kappa\sigma_0, \end{aligned} \right\}, \quad (37)$$

whereas from (33), (33A) we find

$$r - w = z\kappa\sigma_0. \quad (37A)$$

In order that these two equations should be consistent, we must have

$$\sigma_0 = \rho. \quad (38)$$

This is the *condition for the Curie point*. At high temperatures,  $\rho > \sigma_0$ , because  $\rho$  must be positive and  $\sigma_0$  vanishes for  $T = \infty$ . (At  $T = \infty$   $\rho$  has

the value  $1/z$ .) At low temperatures,  $\rho < \sigma_0$ , because  $p_n$  is only large for very small  $n$ . For the simple cubic lattice, the condition (38) is fulfilled for

$$x_0 = 0.6563,$$

corresponding to  $\Theta = 2.372 \text{ V}/k$ , whereas in the first approximation (6) we find  $x_0 = 0.6667$ . The Curie point is therefore slightly lowered by the improvement in the approximation.

By taking higher powers in  $\kappa$  into account,  $\kappa$  can be determined as a function of temperature. A quadratic equation is obtained in this way, viz.,

$$\begin{aligned} \kappa^2 \sum_n \left\{ \left(1 - \frac{2n}{z}\right)^4 - \left(1 - \frac{2n}{z}\right)^3 + \frac{1}{2} \frac{(1+x_0)^2}{(\frac{1}{2}z-1)(1+x_0)^2 + 1+x_0^2} \right. \\ \left. \times \frac{2m}{z} \left[ \left(1 - \frac{2n}{z}\right)^2 - \left(1 - \frac{2n}{z}\right) \right] \right\} p_n = \sigma_0 - \rho, \quad (39) \end{aligned}$$

therefore

$$\kappa^2 \approx \sigma_0 - \rho \approx \Theta - T.$$

## 9—RESULTS

For the simple cubic lattice, we find (in second approximation)

$$\kappa^2 = 35.7 (x_0 - x)$$

$$S = \frac{r-w}{r+w} = 3\kappa\sigma_0 = \sqrt{19.45(x_0 - x)} = 2.32 \sqrt{\frac{\Theta - T}{\Theta}},$$

$$\sigma_T - \sigma_0 = 24.60\%,$$

and for the specific heat

$$\left. \begin{array}{l} c_v = 2.14k \text{ just below} \\ c_v = 0.203k \text{ just above} \end{array} \right\} \text{the critical temperature.}$$

The transition point is therefore a little more marked than in the first approximation, the "distant order"  $S$  increases more rapidly below  $\Theta$  and so does the "order of neighbours"  $\sigma$ , which causes a slightly (12%) larger specific heat.

The order has been calculated numerically for various temperatures. The result is given in figs. 4 to 6, which all refer to a simple cubic lattice. Fig. 4 gives the "order of neighbours" as a function of temperature for various approximations, viz.,

- (a) for the linear chain approximation (equation (4));
- (b) for the second approximation with no long-distance order (§ 5);

- (c) for the approximation of Bragg and Williams;
- (d) and (e) for the first and second approximation with order at long distances (§§ 6 and 8).

Fig. 5 gives the long-distance order according to the approximations *c*, *d*, *e*, fig. 6 the specific heat. The latter is seen to increase near the Curie point with improving approximation.

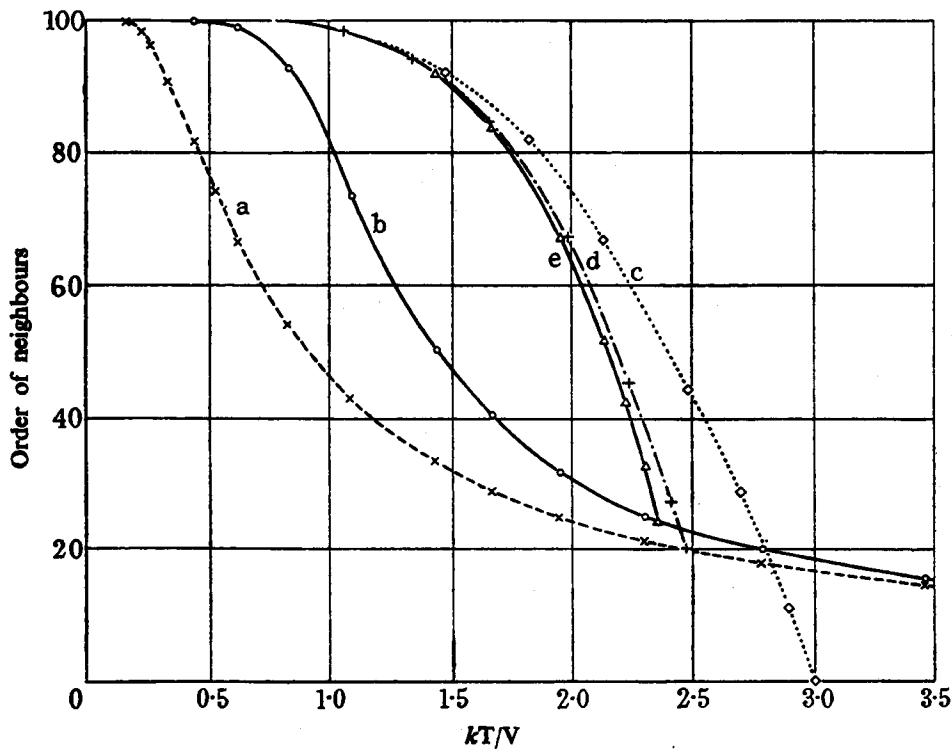


FIG. 4

The results may be checked to some extent by the following method.

It is known that the total energy of any statistical system is connected with its total partition function *P* by

$$E = - \frac{d \log P}{d(1/kT)}. \quad (40)$$

Now, for  $T = 0$  the p.f. (partition function) is 2, corresponding to the two perfectly ordered states of the crystal which have energy zero ( $S = 1$  and  $S = -1$ ). For  $T = \infty$ , the energy is irrelevant, therefore the contribution of each state of the crystal to the p.f. is 1. The  $\frac{1}{2}N$  A-atoms

and the  $\frac{1}{2}N$  B-atoms may be distributed in any arbitrary way over the  $N$  lattice points, that gives

$$\binom{N}{\frac{1}{2}N} \sim 2^N$$

different distributions. Therefore

$$\log S_{T=\infty} = N \log 2; \quad \log S_{T=0} = 0 \quad (41)$$

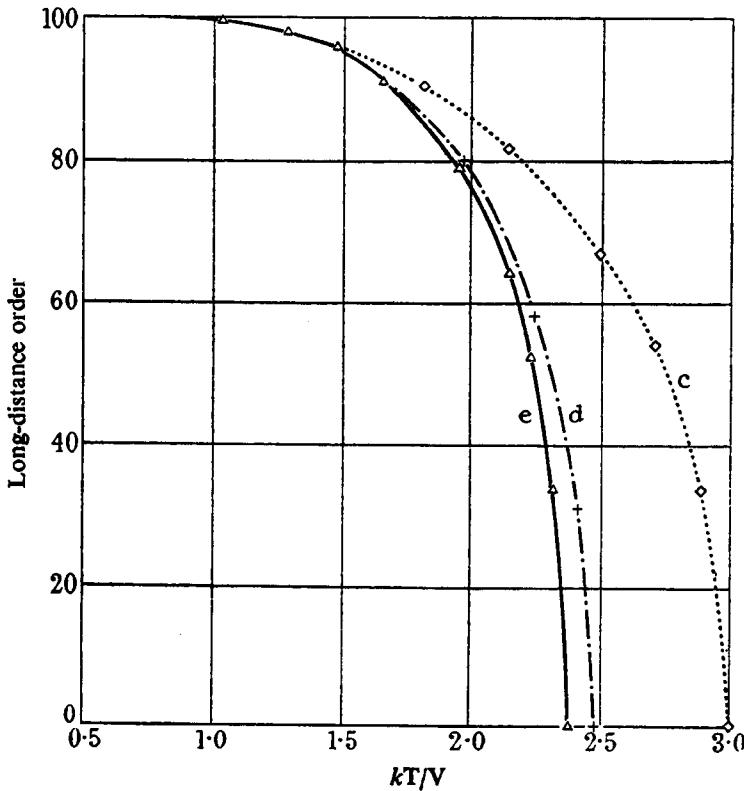


FIG. 5

and (40) becomes

$$\int_0^\infty E(T) d(1/kT) = S_{T=\infty} - S_{T=0} = N \log 2$$

which gives with (1) and (3)

$$\int_0^1 \frac{dx}{x} (1 - \sigma) = \frac{4}{z} \log 2. \quad (42)$$

In our case,  $z = 6$ , so that the right-hand side of equation (42) is 0.462. The left-hand side is 0.465 if the final results of § 8 are inserted, whereas

the approximation of § 5 gives a result 50% too high. The small difference between the "first approximation," considering long-distance order, and the second also seems to show that the final approximation is rather good.

I wish to thank Professor W. L. Bragg very much for suggesting this problem and for many discussions. My special thanks are due to my friend Dr. Peierls, who gave innumerable valuable suggestions. In fact, the method of approximation outlined in § 5 is entirely due to him, and all improvements of the calculation were done on similar lines.

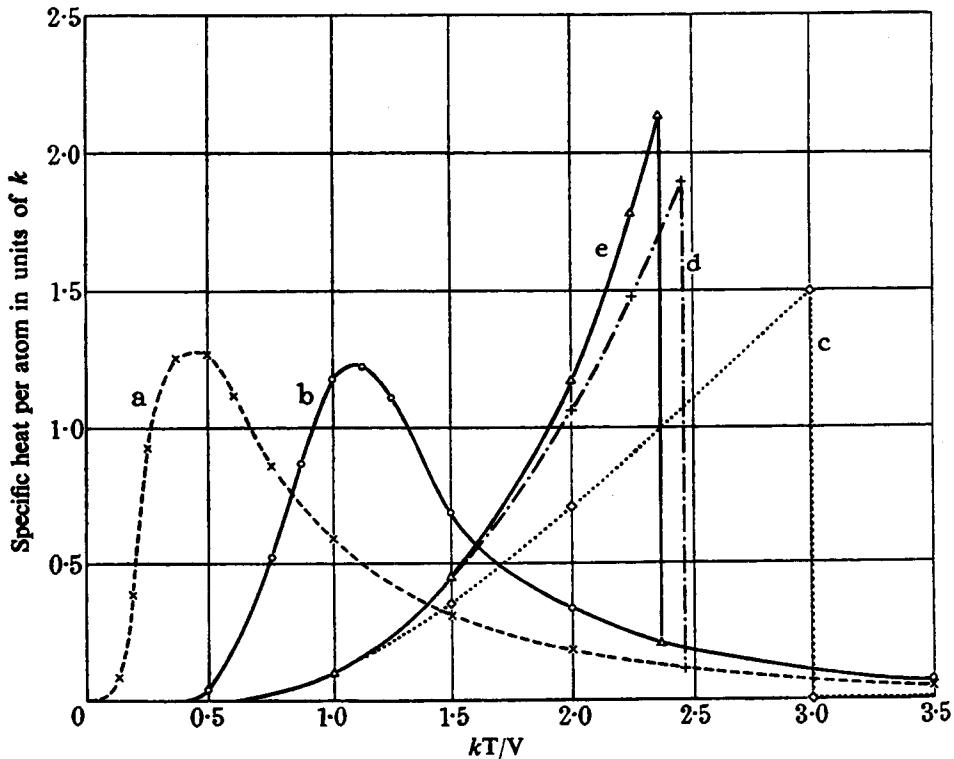


FIG. 6

### SUMMARY

The order in an alloy containing two sorts of atoms in equal proportion is calculated statistically, assuming interaction only between nearest neighbours. At high temperatures, there is only a correlation between near atoms, the state of the crystal as regards order is similar to a liquid.

At low temperatures, the crystal as a whole is ordered, the structure is "solid-like." This order at long distances is restricted to two or more dimensions.\*

The long-distance order and the energy as functions of temperature are both discussed qualitatively (§ 4) and calculated (§§ 6 to 9). It is shown that the theory of Bragg and Williams gives a fair first approximation. The long-distance order vanishes (with vertical tangent) at a certain critical temperature  $\Theta$ . All the physical quantities plotted as functions of  $T$  have a kink at  $T = \Theta$  but no jump. This is due to the fact that two "symmetrical" states exist, having the same energy (§ 4). The derivatives of physical quantities, such as the specific heat, have jumps at the critical temperature. The extra specific heat due to the destruction of order is rather large on the low-temperature side of the critical temperature; it is 70% of the ordinary specific heat due to thermal motion of the atoms (provided all atoms of the crystal take part in the transition). On the high-temperature side of  $\Theta$ , it falls to about 10% of this value. Higher above the critical temperature, the specific heat decreases, but not very rapidly.

\* This should be noted in connection with ferromagnetism which is restricted to three dimensions, due to a quantum mechanical effect.

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**Theory of Bremsstrahlung and Pair Production.****I. Differential Cross Section**

(with L. C. Maximon)

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The theory of bremsstrahlung and electron pair production is generalized to arbitrarily large atomic number  $Z$ , i.e., the Born approximation is avoided. The only assumptions made is that the electron energies involved,  $\varepsilon_1$  and  $\varepsilon_2$ , are large compared with  $mc^2$ . In bremsstrahlung,  $\varepsilon_1$  and  $\varepsilon_2$  are the electron energy before and after emission of the  $\gamma$ -ray. In 1995, Maximon showed that theory is valid for arbitrarily small  $E$ .

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## Theory of Bremsstrahlung and Pair Production. I. Differential Cross Section

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The differential cross sections for bremsstrahlung and pair production are calculated without the use of the Born approximation, assuming the energy of the electron to be large compared to  $mc^2$  both in initial and final state. The wave functions in initial and final state are essentially those previously proposed by Furry (Sec. II). It is proved in Sec. III that our wave functions agree with the exact ones of Darwin except for terms of relative order  $a/l$ , where  $a=Ze^2/\hbar c$  and  $l$  the angular momentum, and that this agreement holds for any energy of the electron. An independent proof is given in Sec. IX, showing that the Furry wave functions give the matrix element correctly except for terms of relative order  $1/e$ .

In the matrix element for bremsstrahlung, the initial state of the electron must be represented by a plane wave plus an outgoing spherical wave, whereas the final state has an ingoing spherical wave (Sec. IV). In pair production, both electrons contain ingoing spherical waves (Sec. V). This causes essential differences between the cross sections for the two processes.

### I. INTRODUCTION AND GENERAL DESCRIPTION OF METHOD

THE exact calculation of bremsstrahlung and pair production is a problem of long standing. For nonrelativistic energies, the bremsstrahlung problem was solved exactly by Sommerfeld.<sup>1</sup> For relativistic energies, a solution has been obtained only in Born approximation, by Bethe and Heitler.<sup>2</sup> The total cross section for pair production by high-energy x-rays has been repeatedly tested by experiment<sup>3-9</sup> and the Bethe-Heitler cross section was found to be correct for light elements, but too high (by about 10 percent) for heavy elements. This discrepancy is less than might have been expected since the error in the Born approximation should be of the order of magnitude  $(Z/137)^2$  which is 36 percent for lead. Still it is reasonable to assume that the discrepancy is due to failure of the Born approximation, and it was attributed to this cause in the experimental papers.

Sommerfeld's success in the nonrelativistic case was due to the fact that the Schrödinger equation for an electron in the Coulomb field can be separated in parabolic coordinates. This provides a wave function for an electron traveling in a definite direction so that, for instance, the problem of Rutherford scattering can

The cross section for pair production is calculated in Sec. VI; the result consists of the Bethe-Heitler formula multiplied by a relatively simple factor, plus another term of similar structure. A simplified derivation is given, which is valid for the important case of small angles between electrons and quantum (Sec. VII); it provides a useful check of the cross section of Sec. VI. In Sec. VIII, the bremsstrahlung cross section is calculated and found to be the Bethe-Heitler result multiplied by a factor. This factor is different from that encountered in pair production and becomes important only for very small momentum transfer  $q$ . In the limit of complete screening, these small  $q$  do not contribute and the cross section goes over into that of the Born approximation.

The error in the cross sections calculated in this paper is estimated (Sec. X) to be of order  $1/e$ , where  $e$  is the energy of the final electron in bremsstrahlung, or that of the less energetic electron in pair production, in units of  $mc^2$ . The total cross section for pair production by a quantum of energy  $k$  may be in error by  $\log k/k$ .

be solved directly and in closed form.<sup>10</sup> This is not possible in relativistic theory, whether Dirac or Klein-Gordon; in this case only a separation in polar coordinates is possible. This makes even the simple problem of electron scattering very cumbersome.<sup>11,12</sup>

If we tried to use wave functions separated in polar coordinates for the bremsstrahlung problem, the calculation would become incredibly cumbersome. We should have to calculate the transition matrix element from any initial angular momentum  $l_1$  of the electron to any final  $l_2$ . Now the important values of  $l$  extend somewhat beyond  $l_0=b/\lambda$ , where  $b$  is the atomic radius and  $\lambda$  the de Broglie wavelength of the electron divided by  $2\pi$ ;  $b/\lambda$  is about  $137e$ , where  $e$  is the electron energy in units of  $mc^2$ , so that for a 100-Mev electron  $l_0$  is nearly 30 000 and the number of matrix elements required about  $10^9$ . Worse than that, in each of these matrix elements the retardation factor for the light quantum,  $e^{ikr}$ , has to be expanded in spherical harmonics, and  $l_2$  terms in this expansion will contribute to the matrix element if  $l_2 < l_1$ . Presumably, these various contributions will interfere partly destructively. The whole calculation would have to be carried out for any pair of initial and final energies,  $\epsilon_1$  and  $\epsilon_2$ . Even if many shortcuts should prove feasible, it is clear that this calculation would be an essentially impossible task.<sup>13</sup>

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<sup>1</sup> A. Sommerfeld, Ann. Physik 11, 257 (1931).

<sup>2</sup> H. A. Bethe and W. Heitler, Proc. Roy. Soc. (London) A146, 83 (1934).

<sup>3</sup> G. P. Adams, Phys. Rev. 74, 1707 (1948).

<sup>4</sup> R. L. Walker, Phys. Rev. 76, 527 (1949).

<sup>5</sup> J. L. Lawson, Phys. Rev. 75, 433 (1949).

<sup>6</sup> DeWire, Ashkin, and Beach, Phys. Rev. 83, 505 (1951).

<sup>7</sup> C. R. Emigh, Phys. Rev. 86, 1028 (1952).

<sup>8</sup> Rosenblum, Schrader, and Warner, Phys. Rev. 88, 612 (1952).

<sup>9</sup> A. I. Berman, Phys. Rev. 90, 210 (1953).

<sup>10</sup> N. F. Mott and H. S. W. Massey, *The Theory of Atomic Collisions* (Clarendon Press, Oxford, 1949), second edition, p. 47.

<sup>11</sup> N. F. Mott and H. S. W. Massey, *The Theory of Atomic Collisions* (Clarendon Press, Oxford, 1949), second edition, p. 74.

<sup>12</sup> W. A. McKinley and H. Feshbach, Phys. Rev. 74, 1759 (1948).

<sup>13</sup> It is true that Harvey Hall, Phys. Rev. 38, 622 (1934), and Revs. Modern Phys. 8, 358 (1936), was able to solve the related problem of the photoelectric effect in the K shell by considering each angular momentum  $l_i$  of the final electron state separately. However, in this case the angular momentum of the initial state

## 769 THEORY OF BREMSSTRAHLUNG AND PAIR PRODUCTION. I

It is therefore essential to find at least an appropriate solution in parabolic coordinates, sufficiently accurate for the calculation of the radiative matrix element. We shall show that a slight modification of Furry's wave function<sup>14</sup> satisfies this condition. Indeed, it will be shown in Sec. III that this wave function is obtained from the exact wave function (i.e., from the expansion in terms of spherical harmonics times radial functions) if in the latter we neglect<sup>15</sup>  $a^2 = (Z/137)^2$  as compared with  $P^2$ . Thus the large values of  $l$  which were disturbing in the solution by expansion in spherical harmonics, turn out to be helpful in this approach. Small values of  $l$  are known to be unimportant: both from the Born approximation solution,<sup>2</sup> and from the Weizsäcker-Williams<sup>16</sup> method, it can be shown that impact parameters less than the Compton wavelength, and thus values of  $l$  less than  $\epsilon$ , give relatively little contribution, the contribution in this region being proportional to  $kd\ell$ . The error due to neglect of  $a^2$  would therefore appear to be of order  $a^2/\epsilon^2$ . Actually, a more detailed consideration of the error in the wave function, along the lines of Sec. III of this paper, shows that the error is of order  $a^2/\epsilon \log \epsilon$ . A similar result,  $a^2/\epsilon$ , will be found from a discussion of the matrix element in Sec. IX. Assuming the latter behavior, the total cross section, integrated over all energies of the final state, will then have an error of order  $a^2\epsilon_1^{-1} \log \epsilon_1$  [see Eq. (10.6)]. Thus our theory will be satisfactory for energies of 50 Mev or more (error less than 2 percent) but will give appreciable errors below 20 Mev.

We propose, then, to use the Furry wave function, which was indeed originally developed for the bremsstrahlung problem. The same wave function, for the same purpose, was developed by Sommerfeld and Maue,<sup>17</sup> but neither they nor Furry used it to calculate the bremsstrahlung itself. The first serious attempt at an exact calculation of bremsstrahlung was made by Bess,<sup>18</sup> who used a wave function of similar structure as Furry's but containing one additional term which Bess believed necessary for the purpose. Unfortunately, as Nordsieck pointed out to us,<sup>19</sup> this additional term is incorrect (see Sec. II) and so is, therefore, Bess' result for the cross section. However, Bess' work is still valuable for the integration of the matrix element and also because he wrote the Furry wave function in a much more convenient form than Furry had done, namely,

$$\psi = Ne^{ip \cdot r} [1 - (i/2\epsilon) \alpha \cdot \nabla] F(ia\epsilon/p; 1; ipr - ip \cdot r), \quad (1.1)$$

is  $l_2=0$  so that only one (actually a few) terms of the expansion of  $e^{ik \cdot r}$  in spherical harmonics contribute. Therefore, at least the individual matrix elements are rather simple; only the summation of the cross section over  $l_1$  is laborious.

<sup>14</sup> W. H. Furry, Phys. Rev. 46, 391 (1934).

<sup>15</sup> This proof goes beyond that of Furry, who had to neglect also terms of order  $1/\epsilon^2$ .

<sup>16</sup> C. F. v. Weizsäcker, Z. Physik 88, 612 (1934); E. J. Williams, Kgl. Danske Videnskab. Selskab. Mat.-fys. Medd. 13, 4 (1935).

<sup>17</sup> A. Sommerfeld and A. W. Maue, Ann. Physik 22, 629 (1935).

<sup>18</sup> L. Bess, Phys. Rev. 77, 550 (1950).

<sup>19</sup> A. Nordsieck (private communication).

where  $p$  is the momentum of the electron in units of  $mc$ ,  $\epsilon = (P^2 + 1)^{1/2}$  its energy in units of  $mc^2$ ,  $a = Ze^2/\hbar c$ ,  $\alpha$  the Dirac operator,  $r$  the electron's coordinate in units of  $\hbar/mc$ , and  $N$  a normalization factor. The derivation of (1.1) will be given in Sec. II (see also Secs. III and IX), and we shall use the wave function in this form for both initial and final state.

The matrix element to be calculated is

$$M = \int \psi_2^* \alpha_\lambda \psi_1 e^{-ik \cdot r} d\tau, \quad (1.2)$$

where  $\lambda$  is the direction of polarization of the light wave,  $\alpha_\lambda$  the Dirac  $\alpha$  matrix in this direction, and the subscripts 1 and 2 refer to initial and final state of the electron. Using (1.1) and neglecting certain terms discussed in Sec. IX, the integral may then be written in the form (6.2), (6.3). (See Sec. VI.) Now the integrals in (6.3) can be evaluated exactly, which is done in Sec. VI, and all other contributions to  $M$  can be neglected as is shown in Sec. IX.

It is somewhat surprising that the three terms in (6.2) are all of the same order of magnitude, whereas it might be expected that the term 1 in the wave function (1.1) would give a much greater contribution than the term  $(i/2\epsilon) \alpha \cdot \nabla$  which at least seems to be of relative order  $1/\epsilon$ . In other words,  $I_1$  of (6.3) may be expected to be much larger than  $I_2$  and  $I_3$ . This is indeed the case, as is shown in Sec. VI and VII;  $I_1$  is of order  $\epsilon$ ,  $I_2$  and  $I_3$  of order 1. Nevertheless, the three integrals give contributions of the same order to the matrix element  $M$ . This is due to the matrix factors in (6.2): the matrix  $(\psi_2^* \alpha_\lambda \psi_1)$  is of order  $1/\epsilon$  whereas the matrix vector  $(\psi_2^* \alpha_\lambda \alpha \psi_1)$  has a component of order unity. This makes the contributions of  $I_1$ ,  $I_2$  and  $I_3$  all of order unity.

The statement about the order of magnitude of the matrix factors can be seen as follows: In the first term of (6.2), the matrix factor  $(\psi_2^* \alpha_\lambda \psi_1)$  represents essentially the velocity of the electron (in units of  $c$ ) perpendicular to the direction of propagation of the quantum,  $k$ . But the differential cross section is known to be large only if the angles  $\theta_1$ ,  $\theta_2$  between the electron directions  $p_1$ ,  $p_2$  and the quantum  $k$  are small, of order  $1/\epsilon$ . Then the electron velocities perpendicular to  $k$  will also be small of this order, and so will the matrix factor  $(\psi_2^* \alpha_\lambda \psi_1)$ . On the other hand, in the second and third term in (6.2), we may, for instance, choose the component of the vector  $\alpha$  in the direction  $\lambda$ . This makes the matrix factor equal to  $(\psi_2^* \alpha_\lambda \psi_1)$  and this is nearly equal to unity because the electron momenta in states 1 and 2 are nearly parallel. This proves the statement above. This fact that  $I_2$  and  $I_3$  give contributions of the same order as  $I_1$ , although they look at first sight much smaller, has been a major cause for obscuring this entire problem in the past.

The contributions to the matrix element  $M$  which are not contained in (6.2) might be expected to fall into three classes: (a) terms which contain an integral of

order 1, and a matrix factor of order  $1/\epsilon$ , (b) terms containing an integral of order  $1/\epsilon$  and a matrix factor of order 1, and (c) terms of order  $\epsilon^{-2} \log \epsilon$  or smaller. The term which Bess tried to take into account<sup>20</sup> is of type (a), as is shown in Sec. IX-c. Examination shows that there is no term of type (b). The term  $\nabla F_2^* \nabla F_1$  which naturally must occur is of type (c) and is shown to be small of order  $\epsilon^{-2} \log \epsilon$  in Sec. IX-d; this term could not easily be evaluated by analytical methods. Generally, the proof that (6.2) determines the matrix element with sufficient accuracy, is given in Sec. IX, and we regard this proof as a central part of our calculation. The most important consequence of this proof is that it is unnecessary to calculate the wave function to a better accuracy than the Furry wave function.

Once the Furry wave function is established as sufficient, the evaluation of the matrix elements is possible using the method of Bess or a similar one of Nordsieck. The resulting differential cross section differs from that of Bess only by the correction of minor algebraic mistakes and the omission of terms arising from the spurious term in Bess' wave function. It is therefore simpler than that of Bess and more similar to the Bethe-Heitler cross section.

In the accompanying paper by Davies and ourselves, the differential cross section is integrated over angles and furthermore it is shown that screening can be taken into account easily.

## II. WAVE FUNCTION

We start with the first-order Dirac equation for an electron in a Coulomb field,

$$(E + Ze^2/\rho)\psi = \beta mc^2\psi - i\hbar c\alpha \cdot \nabla \psi. \quad (2.1)$$

Introducing  $\hbar/mc$  as the unit of length,  $mc^2$  as that of energy,  $a = Ze^2/\hbar c$  and the other notations as described below Eq. (1.1), we get

$$(\epsilon + a/r - \beta + i\alpha \cdot \nabla_r)\psi = 0, \quad (2.2)$$

where  $\nabla_r$  denotes the gradient with respect to the coordinate  $r$ , no longer with respect to  $\rho = (\hbar/mc)r$  as in (2.1). In (2.2),  $\psi$  is the usual four-row unicolumnar matrix, and  $\alpha$  and  $\beta$  the four-row four-column matrices of the Dirac equation.

Since we wish to derive wave functions which are the relativistic generalization of the exact solution of the Schrödinger equation with a Coulomb potential, we transform (2.2) into a second-order equation which reduces to the Schrödinger equation when spin and relativity effects are neglected, i.e., for  $a \ll 1$  and  $r \ll c$ . This may be accomplished by applying the operator  $[(\epsilon + a/r) + \beta - i\alpha \cdot \nabla_r]$  to (2.2), which results in

$$[\nabla_r^2 + p^2 + 2ea/r]\psi = [i\alpha \cdot \nabla_r(a/r) - a^2/r^2]\psi, \quad (2.3)$$

after making use of the commutation relations for  $\alpha$  and

$\beta$ . Here  $p$  is the momentum of the electron in units of  $mc$  and  $p^2 = p^2 + 1$ . The terms on the right-hand side of (2.3) are negligible for  $a \ll 1$  and  $r \ll c$ , in which case we are left with the Schrödinger equation

$$[\nabla_r^2 + p^2 + 2ea/r]\psi = 0. \quad (2.4)$$

As is well known,<sup>1,10</sup> the exact solution of this is

$$\psi = Ne^{ipr} uF, \quad (2.5)$$

where  $N$  is a normalization constant,  $F$  is the confluent hypergeometric function

$$F = F(ia\epsilon/p; 1; ipr - ip \cdot r), \quad (2.6)$$

and  $u = u(p)$ , the normalized Dirac matrix coefficient for a free electron of momentum  $p$ . This factor, which is independent of  $r$ , is the only one by which (2.5) differs from the purely nonrelativistic solution; it insures that (2.5) satisfies also the first order Eq. (2.2) asymptotically for large  $r$ . The asymptotic behavior of (2.5), (2.6) is a plane wave plus outgoing spherical waves.

Following Bess<sup>18</sup> and starting with the wave function  $Ne^{ipr} uF$ , we try to find a solution of the form

$$\psi = Ne^{ipr}(1 + \Omega)uF, \quad (2.7)$$

where  $\Omega$  is an operator to be determined. Then, remembering that (2.5) is an exact solution of (2.4), substitution of (2.7) in (2.3) gives

$$\begin{aligned} & [\nabla_r^2 + 2ip \cdot \nabla_r + 2ea/r]\Omega uF \\ & = [ia\alpha \cdot \nabla_r(1/r) - a^2/r^2](1 + \Omega)uF. \end{aligned} \quad (2.8)$$

If we now assume that  $\Omega$  commutes with the operator  $\nabla_r^2 + 2ip \cdot \nabla_r$ , then (2.8) becomes

$$\begin{aligned} & (2ea/r)\Omega uF - \Omega(2ea uF/r) \\ & = [ia\alpha \cdot \nabla_r(1/r) - a^2/r^2](1 + \Omega)uF. \end{aligned} \quad (2.9)$$

Since the simplest operators that commute with  $\nabla_r^2 + 2ip \cdot \nabla_r$  are those which are made up of any number of differentiations with respect to  $x, y, z$  and of Dirac matrices, we assume  $\Omega$  to be of the form

$$\Omega = \sum_n \sigma_n,$$

where

$$\begin{aligned} \sigma_0 &= a_{01}, \\ \sigma_1 &= a_{11}\partial/\partial x + a_{12}\partial/\partial y + a_{13}\partial/\partial z, \\ \sigma_2 &= a_{21}\partial^2/\partial x^2 + a_{22}\partial^2/\partial y^2 + \dots + a_{24}\partial^2/\partial x\partial y + \dots, \end{aligned} \quad (2.10)$$

and the  $a_{nm}$  are constants or Dirac matrices. In particular,  $\sigma_0$  would merely affect the asymptotic behavior of the wave function. However, since  $u(p)$  is already the correct asymptotic Dirac amplitude,  $\sigma_0$  must not contain any Dirac operators, but must merely be a constant, and as such can be absorbed in the normalizing factor  $N$ . Therefore we may set  $\sigma_0 = 0$  and find that  $\Omega$  contains at least one differentiation with respect to coordinates.

\* With the incorrect wave function used by Bess, this term appeared to be of order 1 instead of  $1/\epsilon$ .

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Substituting (2.10) in (2.9) we may attempt to satisfy (2.9) to terms of  $O(1/r^2)$ , and hence obtain

$$\begin{aligned} -2ea[\sigma_1(1/r)]uF \\ = [ia\alpha \cdot \nabla_r(1/r) - a^2/r^2]uF + O(1/r^3). \end{aligned} \quad (2.11)$$

Mere inspection shows that if we set

$$\sigma_1 = -ia\alpha \cdot \nabla_r/2\epsilon, \quad (2.12)$$

then the first of the terms on the right is canceled. Furthermore, it may be noted that there is no  $\sigma_1$  of the form assumed in (2.10) such that  $\sigma_1(1/r) \sim 1/r^2$ , and thus we cannot satisfy (2.3) to  $O(1/r^2)$  with  $\Omega$  of the form assumed in (2.10).<sup>21</sup> Actually, as will be shown in Sec. IX, it is unnecessary to solve (2.3) with the term involving  $a^2/r^2$  on the right; the solution so far obtained, i.e., with  $\Omega = \sigma_1$  as given in (2.12), is sufficient.

We consider now the wave function  $N e^{ip \cdot r}(1+\Omega)uF$ , where  $\Omega = -(i/2\epsilon)\alpha \cdot \nabla_r$ , and see to what extent it satisfies (2.3), forgetting that we were led to  $\Omega$  by consideration of the terms in (2.9) which contain the lowest power of  $1/r$ . Denoting the wave function that satisfies (2.3) exactly by  $\psi$ , we may write

$$\psi = \psi_a + \psi_b + \psi_c, \quad (2.13)$$

where

$$\psi_a = N e^{ip \cdot r} uF, \quad (2.14)$$

$$\psi_b = -(i/2\epsilon)N e^{ip \cdot r} \alpha \cdot \nabla_r uF, \quad (2.15)$$

and  $\psi_c$  remains undetermined. Thus we wish to see how satisfactory  $\psi_b$  is as a correction to  $\psi_a$ , i.e., to what extent we can neglect  $\psi_c$ . Substituting (2.13), (2.14), (2.15) in (2.3) and noting that

$$[\nabla_r^2 + p^2 + 2ea/r]\psi_a = 0, \quad (2.16)$$

we have

$$\begin{aligned} [\nabla_r^2 + p^2 + 2ea/r](\psi_b + \psi_c) \\ = [ia\alpha \cdot \nabla_r(1/r) - a^2/r^2](\psi_a + \psi_b + \psi_c). \end{aligned} \quad (2.17)$$

Substituting (2.15) and using (2.16), we find

$$[\nabla_r^2 + p^2 + 2ea/r]\psi_b = ia\alpha \cdot \nabla_r(1/r)\psi_a, \quad (2.18)$$

so that

$$\begin{aligned} [\nabla_r^2 + p^2 + 2ea/r]\psi_c &= ia\alpha \cdot \nabla_r(1/r)(\psi_b + \psi_c) \\ &\quad - (a^2/r^2)(\psi_a + \psi_b + \psi_c). \end{aligned} \quad (2.19)$$

We shall return to (2.19) in Sec. IXc when showing that the contribution to the differential cross section coming from  $\psi_c$  may be neglected when compared with that arising from  $\psi_a$  and  $\psi_b$ .

### III. COMPARISON OF THE WAVE FUNCTION WITH THE SOLUTION IN RADIAL WAVES

In this section, we intend to show that our solution to the wave equations (2.14, 2.15) agrees with the

<sup>21</sup> It should be noted that Bess, in the paper referred to, assumes that (2.9) is satisfied to  $O(1/r^2)$  by choosing  $\sigma_1 = -(i/2\epsilon)\alpha \cdot \nabla_r + (a/2\epsilon)\partial/\partial r$ . As pointed out by Dr. Nordström this is incorrect, for although  $(a/2\epsilon)\partial/\partial r(2ea/r) = -a^2/r^2$ , the operator  $\partial/\partial r$  does not commute with  $\nabla_r^2 + 2ip \cdot \nabla_r$ .

exact solution within terms of the order  $a^2/p$  for any energy. Since the matrix element of bremsstrahlung comes mostly from impact parameters equal to  $\hbar/mc$  or larger, the values of  $l$  contributing most are of order  $\epsilon$  or greater. Therefore, the calculations in this section give an added proof that the error in our cross section becomes negligible for large  $\epsilon$ .

The exact solution of the Dirac equation in a Coulomb field has been given by Darwin<sup>22</sup> in the form of an infinite series. Starting from the Darwin solution, Furry<sup>24</sup> has derived wave functions in closed form by neglecting, in each of the terms of the summation, terms of  $O(1/\epsilon^2)$  and of  $O(a^2/p^2)$  compared to those kept, where  $l$  is the angular momentum. We shall show that the wave function which we have been using here, namely  $\psi_a + \psi_b$ , Eq. (2.14, 2.15), may be obtained directly from the Darwin solution by neglecting only terms of  $O(a^2/p)$  in the infinite series, not those of  $O(1/\epsilon^2)$ . Thus the wave function  $\psi_a + \psi_b$  is actually valid for all energies, and, moreover, satisfies [up to terms of  $O(a^2/p)$ ] the more restrictive first-order Dirac equation as well as the second-order equation.

Since the Darwin solution is given as an expansion in spherical harmonics, we shall first expand  $\psi_a + \psi_b$  in spherical harmonics and then show that, apart from a different normalization factor, this is identical with Darwin's series solution when one neglects terms of  $O(a^2/p)$  in the latter. We shall indicate the steps for the initial state wave function; the procedure for the final state is identical.

From the work of Gordon<sup>23</sup> we have, directly,

$$\psi_a = N e^{ip \cdot r} uF = u \sum_l (2l+1) i^l L_l(r) P_l(\cos\theta), \quad (3.1)$$

where

$$L_l(r) = e^{ipr} [\Gamma(l+1-ia_1)/(2l+1)!] (2pr)^l \times e^{ipr} F(l+1-ia_1; 2l+2; -2ipr), \quad (3.2)$$

and

$$a_1 = a\epsilon/p = Ze^2/\hbar v. \quad (3.3)$$

Solving (3.1) for  $uF$  and substituting in  $\psi_b$ , Eq. (2.15), we obtain

$$\begin{aligned} \psi_b &= -\frac{ia\epsilon u}{2\epsilon} \sum_l i^l e^{ipr} \frac{(2l+1)\Gamma(l+1-ia_1)}{(2l+1)!} (2pr)^l e^{ipr} \\ &\quad \times \{\cos\theta P_l[iipF(l+1-ia_1; 2l+2; -2ipr) \\ &\quad + (l/r)F(l+1-ia_1; 2l+2; -2ipr) \\ &\quad - 2ip[(l+1-ia_1)/(2l+2)] \\ &\quad \times F(l+2-ia_1; 2l+3; -2ipr)] \\ &\quad + (\sin\theta/r)P_l^{(1)}F(l+1-ia_1; 2l+2; -2ipr) \\ &\quad - ipP_lF(l+1-ia_1; 2l+2; -2ipr)\} \end{aligned}$$

(continued on next page)

<sup>22</sup> C. G. Darwin, Proc. Roy. Soc. (London) A118, 654 (1928).

<sup>23</sup> W. Gordon, Z. Physik 48, 180 (1928).

$$\begin{aligned}
& -i(\alpha_x \cos \varphi + \alpha_y \sin \varphi)(u/2\epsilon) \sum i^l e^{i\pi a_1} (2l+1) \\
& \times [\Gamma(l+1-i\alpha_1)/(2l+1)!] (2pr)^l e^{i\pi r} \\
& \times \{\sin \theta P_l[i\dot{p}F(l+1-i\alpha_1; 2l+2; -2ipr) \\
& + (l/r)F(l+1-i\alpha_1; 2l+2; -2ipr) \\
& - 2ip[(l+1-i\alpha_1)/(2l+2)] \\
& \times F(l+2-i\alpha_1; 2l+3; -2ipr)] - (\cos \theta/r)P_l^{(1)} \\
& \quad \times F(l+1-i\alpha_1; 2l+2; -2ipr)\}, \quad (3.4)
\end{aligned}$$

where we have defined  $P_l^{(1)} = \sin \theta (dP_l/d\cos \theta)$ , and note that  $\alpha \cdot r = \alpha_x \sin \theta \cos \varphi + \alpha_y \sin \theta \sin \varphi + \alpha_z \cos \theta$  and  $\alpha \cdot p = \alpha_x \dot{p}$ , since the  $z$  axis has been chosen in the direction of  $p$ .

In order to obtain an expansion of  $\psi_b$  in spherical harmonics, we make use of the following recurrence relations involving the Legendre polynomials  $P_l$  and the associated Legendre functions  $P_l^{(1)}$ :

$$\begin{aligned}
\sin \theta P_l^{(1)} &= l[P_{l-1} - \cos \theta P_l], \\
(2l+1) \sin \theta P_l &= P_{l+1}^{(1)} - P_{l-1}^{(1)}, \\
(2l+1) \cos \theta P_l &= (l+1)P_{l+1} + lP_{l-1}, \\
(2l+1) \cos \theta P_l^{(1)} &= lP_{l+1}^{(1)} + (l+1)P_{l-1}^{(1)},
\end{aligned} \quad (3.5)$$

in which we define  $P_0^{(1)} = 0$  and  $P_{-1}^{(1)} = 0$  in order that these recurrence relations will also be valid for  $l=0$ . We also make use of the following recurrence relations for the confluent hypergeometric function:

$$\begin{aligned}
xF(a+1; b+1; x) &= b[F(a+1; b; x) - F(a; b; x)], \\
xaF(a+1; b+1; x) &= b(b-1)[F(a; b-1; x) \\
&\quad - F(a; b; x)], \quad (3.6) \\
aF(a+1; b+1; x) &= (a-b)F(a; b+1; x) \\
&\quad + bF(a; b; x).
\end{aligned}$$

The last of these three relations can be derived directly from the first two.

By straightforward but tedious application of (3.5) and (3.6), we may obtain

$$\begin{aligned}
\psi_b &= (\alpha_1/2\epsilon)\alpha_x u \sum e^{i\pi a_1} (2l+1) i^l \\
&\times [\Gamma(l+1-i\alpha_1)/(2l+1)!] (2pr)^l (e^{i\pi r}/r) P_l \\
&\times [F(l+1-i\alpha_1; 2l+2; -2ipr) \\
&+ i\alpha_1(l-i\alpha_1)^{-1} F(l-i\alpha_1; 2l+2; -2ipr)] \\
&+ (\alpha_1/2\epsilon)(\alpha_x \cos \varphi + \alpha_y \sin \varphi) u \sum e^{i\pi a_1} \\
&\times (2l+1)i^l [\Gamma(l+1-i\alpha_1)/(2l+1)!] \\
&\times (2pr)^l (e^{i\pi r}/r) P_l^{(1)} (l-i\alpha_1)^{-1} \\
&\quad \times F(l-i\alpha_1; 2l+2; -2ipr). \quad (3.7)
\end{aligned}$$

Having obtained the expansions of  $\psi_a$  and  $\psi_b$  in spherical harmonics, we turn now to the Darwin solution as given in Mott and Massey,<sup>24</sup> where the following

<sup>24</sup> N. F. Mott and H. S. W. Massey, *The Theory of Atomic Collisions* (Clarendon Press, Oxford, 1949), second edition, p. 76, Eq. (25); p. 79, Eqs. (35), (37), and (38).

two components of the wave function are given:

$$\begin{aligned}
\psi_3 &= \sum [(l+1)e^{i\pi} G_l + le^{i\pi-l-1} G_{-l-1}] i^l P_l, \\
\psi_4 &= \sum [-e^{i\pi} G_l + e^{i\pi-l-1} G_{-l-1}] i^l P_l^{(1)} e^{i\pi}, \quad (3.8)
\end{aligned}$$

where

$$\begin{aligned}
e^{i\pi-l-1} G_{-l-1} &= \frac{\Gamma(\rho_l+1-i\alpha_1) i e^{i\pi a_1} e^{i\pi(l-\rho_l)}}{2\Gamma(2\rho_l+1)(\rho_l-i\alpha_1)} \frac{(2pr)^{\rho_l}}{pr} \\
&\times \{-(l-i\alpha_1/\epsilon)F(\rho_l-i\alpha_1; 2\rho_l+1; -2ipr) \\
&+ (\rho_l-i\alpha_1)F(\rho_l+1-i\alpha_1; 2\rho_l+1; -2ipr)\}, \quad (3.9)
\end{aligned}$$

and  $\rho_l = (l^2 - a^2)^{1/2}$  (positive square root implied).  $e^{i\pi} G_l$  may be obtained directly from (3.9) by replacing  $l$  by  $-l-1$  everywhere except in the factor  $e^{i\pi(l-\rho_l)}$  which is replaced by  $e^{i\pi(l-\rho_l-1)}$ . In obtaining (3.9) from Mott and Massey, we have replaced  $n$ ,  $\alpha = Ze^2/hc$ ,  $\gamma = Ze^2/hv$ , and  $\gamma' = \gamma(1-v^2/c^2)^{1/2}$ , by their corresponding symbols in the notation that we have been using, namely  $l$ ,  $a$ ,  $a_1$ , and  $a_1/\epsilon$ , respectively. We have also divided  $G_{-l-1}$  and  $G_l$  (as given in Mott and Massey) by  $p$  in order that they have the same asymptotic behavior as  $L_l(r)$ , given in (3.1). Further, the relation

$$F(a; b; x) = e^x F(b-a; b; -x)$$

has been substituted in the Darwin solution in order that the arguments of the confluent hypergeometric functions be the same as those in (3.1) and (3.2) for  $\psi_a$  and  $\psi_b$ .

If we assume  $a^2/l^2 \ll 1$  in each term of the sum, then  $\rho_l$  and  $\rho_{-l-1}$  may be replaced by  $l$  and  $l+1$ , respectively, so that we have then, from (3.9),

$$\begin{aligned}
e^{-i\pi-l-1} G_{-l-1} &= \frac{i \Gamma(l+1-i\alpha_1) e^{i\pi a_1}}{2 \Gamma(2l+1)(l-i\alpha_1)} \frac{(2pr)^l}{pr} \\
&\times \{-(l-i\alpha_1/\epsilon)F(l-i\alpha_1; 2l+1; -2ipr) \\
&+ (l-i\alpha_1)F(l+1-i\alpha_1; 2l+1; -2ipr)\}, \quad (3.10).
\end{aligned}$$

and

$$\begin{aligned}
e^{i\pi} G_l &= \frac{\Gamma(l+2-i\alpha_1) e^{i\pi a_1}}{2\Gamma(2l+3)(l+1-i\alpha_1)} \frac{(2pr)^l}{pr} \\
&\times \{(l+1+i\alpha_1/\epsilon)F(l+1-i\alpha_1; 2l+3; -2ipr) \\
&+ (l+1-i\alpha_1)F(l+2-i\alpha_1; 2l+3; -2ipr)\}. \quad (3.11)
\end{aligned}$$

By substituting (3.10) and (3.11) in (3.8) we may obtain, after numerous applications of the relations given in (3.6),

$$\begin{aligned}
\psi_3 &= \sum (2l+1)(2l+1)!^{-1} i^l e^{i\pi a_1} \Gamma(l+1-i\alpha_1) (2pr)^l \\
&\quad + e^{i\pi r} F(l+1-i\alpha_1; 2l+2; -2ipr) P_l \\
&\quad + (a_1 p/2\epsilon)(\epsilon+1)^{-1} \sum (2l+1)(2l+1)!^{-1} i^l e^{i\pi a_1} \\
&\quad \times \Gamma(l+1-i\alpha_1) (2pr)^l (e^{i\pi r}/r) P_l^{(1)} \\
&\quad \times \{F(l+1-i\alpha_1; 2l+2; -2ipr) \\
&\quad + i\alpha_1(l-i\alpha_1)^{-1} F(l-i\alpha_1; 2l+2; -2ipr)\}, \quad (3.12)
\end{aligned}$$

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and

$$\begin{aligned}\psi_4 = & (a_1 p / 2\epsilon) (\epsilon + 1)^{-1} e^{ipr} \sum (2l+1)(2l+1)!^{-1} i^l e^{i\pi a_1} \\ & \times \Gamma(l+1-i a_1) (2pr)^l (e^{ipr}/r) P_l^{(1)} \\ & \times (l-i a_1)^{-1} F(l-i a_1; 2l+2; -2ipr). \quad (3.13)\end{aligned}$$

We note first that, apart from the matrix factors, the terms in the summation for  $\psi_3$  [Eq. (3.12)] are identical to those in (3.1) for  $\psi_a$  and in (3.7) for the part of  $\psi_b$  with the factor  $a_s$ . Further, apart from the matrix factors, the terms in the summation for  $\psi_4$  (Eq. (3.13)) are identical to those with the factors  $a_z$  and  $a_s$  in the summation for  $\psi_b$  in (3.7).

Now, if  $u$  represents the state with positive energy and "spin up," then, since we have chosen the  $z$  axis in the direction of  $p$ , we have  $p_z = p_y = 0$ ,  $p_x = p$ , and

$$u = [1 + p^2 / (\epsilon + 1)^2]^{-\frac{1}{2}} \begin{pmatrix} 1 \\ 0 \\ p / (\epsilon + 1) \\ 0 \end{pmatrix}. \quad (3.14)$$

Thus with

$$\begin{aligned}\alpha_z = & \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}, \quad \alpha_s = \begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \end{pmatrix}, \\ \alpha_x = & \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}, \quad (3.15)\end{aligned}$$

and numbering the Dirac components of our wave function (3.1) by  $\psi_{a1}$ ,  $\psi_{a2}$ ,  $\psi_{a3}$ ,  $\psi_{a4}$ , we have, from (3.1), (3.7), (3.12), and (3.13),

$$\begin{aligned}\psi_{a1} + \psi_{b1} = & [1 + p^2 / (\epsilon + 1)^2]^{-\frac{1}{2}} \psi_1, \\ \psi_{a2} + \psi_{b2} = & [1 + p^2 / (\epsilon + 1)^2]^{-\frac{1}{2}} \psi_2,\end{aligned} \quad (3.16)$$

where  $\psi_3$  and  $\psi_4$  refer to the function of Mott and Massey. The wave function used here,  $\psi_a + \psi_b$ , is, therefore, apart from a difference of normalization factor,<sup>26</sup> identical with that of Darwin after neglecting terms of  $O(a^2/p)$  in the latter.\*

It may be noted that since we have assumed only  $a^2/p \ll 1$  rather than  $a^2 \ll 1$  in each of the terms, further corrections to  $\psi_a + \psi_b$  may be obtained fairly easily. We need only write

$$\psi = \psi^{(1)} + \sum_i [f_i(r, \theta, \phi; a^2) - f_i(r, \theta, \phi; 0)], \quad (3.17)$$

where  $\psi^{(1)}$  is our old solution of Sec. II,  $f_i(r, \theta, \phi; a^2)$  is the component of the exact Darwin solution for a given

\* Darwin, Mott, and Massey, take the particle density to be  $|\psi_1|^2 + |\psi_2|^2$  and consider  $\psi_1$  and  $\psi_2$  as expressed in terms of  $\psi_3$ ,  $\psi_4$ . We take the density to be  $|\psi_1|^2 + |\psi_2|^2 + |\psi_3|^2 + |\psi_4|^2$ ; this explains the difference in normalization.

\* Note added in proof.—Closer examination shows that our wave function (3.2) differs from Darwin's true wave function by terms of order  $a^2/l$  rather than  $a^2/p$ . This will be shown in a forthcoming paper by one of us (L. C. M.). It has the consequence of making the error in our matrix element of order  $a^2/(e \log e)$ , as mentioned in Sec. I.

$l$ , and  $f_i(r, \theta, \phi; 0)$  is the same component with  $a^2/l^2$  replaced by zero. In practice, the sum is extended over a finite number of terms according to the accuracy desired.

## IV. THE MATRIX ELEMENT IN BREMSSTRAHLUNG

It is well known<sup>26</sup> that the matrix element for bremsstrahlung is

$$H_{12}' = C \int \psi_2^* \alpha_\lambda e^{-ik \cdot r} \psi_1 d\tau, \quad (4.1)$$

where

$$C = -e\hbar c(2\pi/k)^{\frac{1}{2}}, \quad (4.2)$$

and  $\alpha_\lambda$  is the component of the Dirac matrix operator  $\alpha$  in the direction of polarization,  $\lambda$ , which is perpendicular to the propagation vector  $\mathbf{k}$ . The wave functions  $\psi_1$  and  $\psi_2$  of the initial and final state of the electron are taken in the Coulomb potential and are given by the expressions in Secs. II and III.

The wave function of a continuum state, however, is not fully defined until its asymptotic behavior is given. In the case of  $\psi_1$ , it is clear that it has to be represented by a plane wave propagating in the direction of the initial momentum  $\mathbf{p}_1$ , plus outgoing spherical waves. In the past,<sup>1,18,27</sup>  $\psi_2$  has often been chosen in the same manner. That this is incorrect was recognized first by Mott and Massey<sup>28</sup> in a more general context and then by Sommerfeld<sup>29</sup> in relation to our particular problem. A physical argument was given by us in an earlier paper.<sup>30</sup> The correct theory was used for internal conversion by Rose *et al.*<sup>31</sup> who give references to several previous papers in which the incorrect assumption was made, as well as to Rarita and Schwinger<sup>32</sup> who were familiar with the correct treatment.

A mathematical argument which leads to that of Mott and Massey is as follows. The Hamiltonian of our system is

$$H = H_e + H_r + H', \quad (4.3)$$

where  $H_r$  is the Hamiltonian of the pure radiation field,  $H_e$  that of the electron including its Coulomb interaction with the nucleus, and  $H'$  the interaction between electron and radiation. The latter is to be regarded as a small perturbation, and to be treated only in first approximation. The Schrödinger equation is

$$H\Psi = E_1\Psi, \quad (4.4)$$

where  $E_1$  is the energy of the incident electron. In zero order, we have no radiation present, and the wave function therefore satisfies

$$H_e\Psi^{(0)} = E_1\Psi^{(0)}. \quad (4.5)$$

<sup>26</sup> See Heitler, *The Quantum Theory of Radiation* (Oxford University Press, London, 1944), second edition, p. 96.

<sup>27</sup> L. Maximon and H. A. Bethe, Phys. Rev. 87, 156 (1952).

<sup>28</sup> Reference 24, pp. 111-13.

<sup>29</sup> A. Sommerfeld, *Atombau und Spektrallinien* (F. Vieweg and Son, Braunschweig, 1939), Vol. 2, pp. 457 and 502.

<sup>30</sup> Bethe, Maximon, and Low, Phys. Rev. 91, 417 (1953).

<sup>31</sup> Rose, Biedenharn, and Arfken, Phys. Rev. 85, 5 (1952).

<sup>32</sup> W. Rarita and J. Schwinger, Phys. Rev. 59, 436 (1941).

The solution of this equation is the initial electron wave function,  $\psi_1$ .

In first order, we have to solve

$$(H_e + H_s - E_1)\Psi^{(1)} = -H'\Psi^{(0)}. \quad (4.6)$$

Now if we take the part of  $\Psi^{(1)}$  in which there is a quantum  $k$  present,  $H_s\Psi^{(1)} = k\Psi^{(1)}$  and

$$(H_e - E_2)\Psi^{(1)} = -H'\Psi^{(0)} = -H'\psi_1, \quad (4.7)$$

since  $E_2 = E_1 - k$ . Now if we take the factor of  $\Psi^{(1)}$  which describes the electron and denote it by  $\phi$ , then

$$(H_e - E_2)\phi = C'\alpha\psi_1 e^{-ik \cdot r} = S, \quad (4.8)$$

where  $C'$  is a constant closely related to  $C$ , Eq. (4.2). The right-hand side of (4.8) will be called "the source" and denoted by  $S$ . Our task is now to solve (4.8) by a wave function  $\phi$  which consists exclusively of outgoing spherical waves, without any plane wave, because there is no incident electron having the final momentum  $p_2$ .

Writing the left-hand side of (4.8) more explicitly, we seek a solution of

$$[\nabla^2 + p_2^2 + U(r)]\phi = S, \quad (4.9)$$

where  $U(r)$  is the "potential operator" occurring in (2.3), *viz.*,

$$U(r) = 2ea/r - i\alpha\alpha \cdot \nabla(1/r) + \alpha^2/r^2, \quad (4.10)$$

and the solution  $\phi$  is supposed to contain only outgoing spherical waves. Exactly the same problem is solved by Mott and Massey, with somewhat different notation and with the restrictive assumption that

$$rU(r) \rightarrow 0, \text{ as } r \rightarrow \infty.$$

This restriction is not satisfied by our potential (4.10) but can be satisfied by introducing a screening factor  $e^{-ar}$  in (4.10) and letting  $a$  go to zero in the end.

Mott and Massey show that  $\phi$  behaves asymptotically, as

$$\phi(r) = -(4\pi r)^{-1}e^{ip_2 \cdot r} \int dr' S(r') \mathfrak{F}(r', \pi - \Theta), \quad (4.11)$$

where

$$\mathfrak{F}(r', \theta) = \sum (2l+1)i^l e^{i\eta_l} L_l(r') P_l(\theta) \quad (4.12)$$

is the well-known solution of the *homogeneous* wave equation in the given potential, *i.e.*, of (4.9) with zero on the right-hand side. The asymptotic behavior of  $\mathfrak{F}$  is the usual one, *viz.*, plane wave plus outgoing spherical waves.  $L_l$  is the regular (and real) solution of the radial wave equation and  $\eta_l$  the phase shift for angular momentum  $l$  in the given potential. According to (4.11),  $\mathfrak{F}$  must be taken in the integrand at the angle  $\pi - \Theta$ , where  $\Theta$  is defined by Mott and Massey as the angle between the vectors  $r$  and  $r'$ . Now we are interested in the asymptotic behavior of  $\phi(r)$  in the direction  $p_2$ ; therefore we must choose  $r$  in (4.11) in the direction of  $p_2$ , and  $\pi - \Theta = \chi$  is the angle between  $-p_2$  and  $r'$ .

Therefore  $\mathfrak{F}(r', \pi - \Theta)$  is a function which behaves asymptotically like a plane wave propagating in the direction  $-p_2$ , plus the outgoing spherical waves associated with it by the potential  $U(r)$ ; thus,

$$\mathfrak{F}(r, \pi - \Theta) \rightarrow e^{ip_2 \cdot r} + r^{-1}e^{ip_2 \cdot r} f(\chi), \quad (4.13)$$

where  $\chi = \pi - \Theta$  is the angle between  $-p_2$  and  $r$ , and  $f(\chi)$  is the amplitude of the wave scattered through an angle  $\chi$  from the direction of the plane wave,  $-p_2$ .

It should be noted that in (4.11)  $\mathfrak{F}$  occurs, not  $\mathfrak{F}^*$ . Therefore  $\mathfrak{F}$  must be identified with  $\psi_2^*$  in the matrix element (4.1). Therefore  $\psi_2$  itself<sup>33</sup> will be

$$\psi_2 = \mathfrak{F}^*(r, \pi - \Theta) = e^{ip_2 \cdot r} + r^{-1}e^{-ip_2 \cdot r} f^*(\chi). \quad (4.14)$$

In other words,  $\psi_2$  is a plane wave propagating as usual in the direction  $+p_2$ , plus a spherical wave which is *ingoing* rather than outgoing. The amplitude of the ingoing wave is large near  $\chi = 0$ , or  $\Theta = \pi$ , *i.e.* on the side *from which the plane wave is coming*, as is reasonable for an ingoing spherical wave associated with the plane wave  $e^{ip_2 \cdot r}$ .<sup>34</sup>

We can prove more explicitly that  $\psi_2$  is just the solution of the homogeneous equation which satisfies the boundary condition of having no *outgoing* spherical waves added to the plane wave  $e^{ip_2 \cdot r}$ . Inserting  $\theta = \pi - \Theta$  in (4.12), we note that  $P_l(\pi - \Theta) = (-1)^l P_l(\Theta)$  and  $i^l(-1)^l = i^{2l}$ ; in fact, this is the way in which  $\mathfrak{F}(r', \pi - \Theta)$  is first introduced in the derivation by Mott and Massey. Therefore

$$\begin{aligned} \psi_2(r') &= \mathfrak{F}^*(r', \pi - \Theta) \\ &= \sum (2l+1)i^l e^{-i\eta_l} L_l(r') P_l(\theta). \end{aligned} \quad (4.15)$$

This differs from the usual expression for the wave function, (4.12), only by having  $e^{-i\eta_l}$  instead of  $e^{i\eta_l}$ . By considering the asymptotic behavior of  $L_l(r')$ , it is easily seen<sup>35</sup> that

$$\psi_2 = e^{ip_2 \cdot r} + r^{-1}e^{-ip_2 \cdot r} g(\theta), \quad (4.16)$$

with

$$\begin{aligned} g(\theta) &= (-2ik)^{-1} \sum (2l+1)(e^{-2i\eta_l} - 1)(-1)^l P_l(\theta) \\ &= f^*(\pi - \theta) = f^*(\chi). \end{aligned} \quad (4.17)$$

For the actual evaluation of the matrix element, it is more convenient to use  $\mathfrak{F}$  than  $\psi_2$ . As is seen from (4.13),  $\mathfrak{F}$  is the usual solution, plane wave plus outgoing spherical waves, only with  $-p_2$  instead of  $+p_2$ . Therefore, if we consider only the part of the matrix element (4.1) arising from the "main" part  $\psi_a$ , defined in (2.13),

<sup>33</sup> There is of course no need to go to  $\psi_2$ ; the actual calculation could be done equally well directly with  $\mathfrak{F}$ .

<sup>34</sup> It is good to note that in the Born approximation one doesn't need to pay attention to the incoming wave because one doesn't consider any spherical waves at all in the wave function. This was recognized by Mott and Massey, p. 356, reference 10.

<sup>35</sup> As in Mott and Massey, pp. 22-24, reference 10.

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of the wave functions  $\psi_1$  and  $\psi_2$ , we get

$$H_{12}' = CN_1 N_2^* (u_2^* \alpha_\lambda u_1) \int d\tau e^{-ik \cdot r} e^{i(p_1 - p_2) \cdot r} \times F(i\epsilon_1; 1; ip_1 r - ip_1 \cdot r) F(i\epsilon_2; 1; ip_2 r + ip_2 \cdot r) \quad (4.18)$$

with

$$a_1 = a\epsilon_1/p_1, \quad a_2 = a\epsilon_2/p_2. \quad (4.19)$$

The usual choice of  $\psi_2$ , with outgoing spherical waves, would replace the last factor in (4.18) by

$$F(-i\epsilon_2; 1; -ip_2 r + ip_2 \cdot r). \quad (4.20)$$

The evaluation of the matrix element will be given in Sec. VIII.

#### V. WAVE FUNCTION AND MATRIX ELEMENT IN PAIR PRODUCTION

In the case of pair production, *both* the electron and the positron are produced, and therefore both should be represented by plane waves with convergent spherical waves. Thus, in contrast to the Born approximation theory, there is a significant difference between the matrix element for bremsstrahlung and pair production. The latter is

$$H_{12}' = C \int \psi_-^* \alpha_\lambda \psi_+^* e^{ik \cdot r} d\tau, \quad (5.1)$$

where  $\psi_+$  is the wave function of the positron.

The spinor factor  $u_+^*$  in the wave function  $\psi_+^*$  of a positron of momentum  $p_+$  is the same as the spinor factor  $u_1$  (not conjugate) in the wave function of an electron of momentum  $-p_+$  and negative energy  $-\epsilon_+$ . The matrix element (5.1) thus contains the matrix factor

$$b = (u_-^* \alpha_\lambda u_1). \quad (5.2)$$

The spatial part of  $\psi_+$  differs from that of an electron by having the sign of the Coulomb interaction reversed. This can be accomplished by changing the sign of  $a\epsilon/p$  in the first argument of the hypergeometric function (2.6), thus obtaining

$$\psi_{+a}' = N_+ e^{ip_+ \cdot r} u_+ F(-i\epsilon_+/p_+; 1; ip_+ r - ip_+ \cdot r) \quad (5.3)$$

for a positron going in the direction  $p_+$  plus *outgoing* spherical waves. For  $\psi_+$  in (5.1) we must again take ingoing spherical waves, so that  $\psi_+^*$  is represented, in analogy with (4.18), by

$$\psi_{+a}^* = N_+^* e^{-ip_+ \cdot r} u_1 F(-i\epsilon_1; 1; ip_+ r + ip_+ \cdot r), \quad (5.4)$$

with

$$a_1 = a\epsilon_+/p_+. \quad (5.5)$$

Similarly, the negaton is described by a wave function  $\psi_-^*$  exactly like the last factor of (4.18), and the "main"

part of the matrix element (5.1) becomes

$$H_{12}' = CN_+^* N_-^* (u_-^* \alpha_\lambda u_1) \int d\tau e^{i(k-p_1-p_2) \cdot r} \times F(-i\epsilon_1; 1; ip_+ r + ip_+ \cdot r) \times F(i\epsilon_2; 1; ip_+ r + ip_+ \cdot r). \quad (5.6)$$

Asymptotically for large  $r$ , the hypergeometric function gives a large scattered wave where its argument is small. The scattered waves of *both* electron and positron in (5.6) are therefore large when  $r$  is in the direction  $-p$  (convergent waves), whereas in (4.18) one scattered wave (for the incident electron) is large in the direction  $+p$ , the other (outgoing electron) in the direction  $-p$ . This will make a considerable difference in the matrix element.

As is well known,  $\psi_+^*$  can also be considered as the wave function (not conjugate) of a negative energy, negatively charged electron. The usual prescription for obtaining this is to take the electron wave function

$$\psi_1 = N_1 e^{ip_1 \cdot r} F(i\epsilon_1/p_1; 1; ip_1 r - ip_1 \cdot r) u(p_1, \epsilon_1), \quad (5.7)$$

and substitute  $\epsilon_1 = -\epsilon_+$ ,  $p_1 = -p_+$ , while leaving  $p_1 = +p_+$ . It is easily seen that this leads to the correct function

$$\psi_1 = N_1 e^{-ip_+ \cdot r} \times F(-i\epsilon_+/p_+; 1; ip_+ r + ip_+ \cdot r) u(-p_+, -\epsilon_+), \quad (5.8)$$

which is exactly the function occurring in (5.6).

#### VI. EVALUATION OF THE PAIR MATRIX ELEMENT AND CROSS SECTION

We proceed now to the evaluation of the matrix element (5.1). For ease of writing, we shall denote the quantities referring to the positron by the subscript 1 rather than +, and those referring to the electron by 2. Thus  $p_1 = p_+$  in the next two sections,  $F_1$  is the hypergeometric function relating to the positron and  $F_2^*$  that for the electron.

We substitute  $d^3\rho = (\hbar/mc)^3 d^3r$  and  $\psi_1 = \psi_{1a} + \psi_{1b} + \psi_{1c}$ , as in (2.13), and similarly for the negaton. Of the resulting integrals we will show that three may be evaluated in closed form, and those remaining will be shown in Sec. IX to give contributions to the differential cross-section which may be neglected when the energies of the positive and negative electron are much larger than  $mc^2$ .

We proceed then to those integrals that may be evaluated in closed form and to the differential cross-section determined from them alone. These integrals are

$$C \int \psi_{2a}^* \alpha_\lambda e^{ik \cdot r} \psi_{1a} d^3\rho + C \int \psi_{2a}^* \alpha_\lambda e^{ik \cdot r} \psi_{1b} d^3\rho + C \int \psi_{2b}^* \alpha_\lambda e^{ik \cdot r} \psi_{1a} d^3\rho. \quad (6.1)$$

Using (2.14), (2.15), the matrix element which we will use may be written in the form

$$H_{12}' = C' [(u_2^* \alpha_\lambda u_1) I_1 + (u_2^* \alpha_\lambda \alpha \cdot I_2 u_1) + (u_2^* \alpha \cdot I_3 \alpha_\lambda u_1)], \quad (6.2)$$

where

$$I_1 = \int e^{i\mathbf{q} \cdot \mathbf{r}} F_2^* F_1 d^3 r, \quad (6.3)$$

$$I_2 = - (i/2\epsilon_1) \int e^{i\mathbf{q} \cdot \mathbf{r}} F_2^* \nabla F_1 d^3 r, \quad (6.3a)$$

$$I_3 = (i/2\epsilon_1) \int e^{i\mathbf{q} \cdot \mathbf{r}} (\nabla F_2^*) F_1 d^3 r, \quad (6.3b)$$

and

$$C' = C(\hbar/mc)^3 N_2^* N_1, \quad (6.4)$$

$$\mathbf{q} = \mathbf{k} - \mathbf{p}_1 - \mathbf{p}_2. \quad (6.5)$$

$N_1$  and  $N_2$  will be determined so that  $\psi_1$  and  $\psi_2$  are normalized to unit amplitude asymptotically. Following Bess again, the integrals in (6.3) may be obtained from the integral

$$I_0 = \int e^{-\lambda r} e^{i\mathbf{q} \cdot \mathbf{r}} F_2^* F_1 d^3 r / r \quad (6.6)$$

by differentiation with respect to parameters. Thus

$$I_1 = - \partial I_0 / \partial \lambda |_{\lambda=0}. \quad (6.7)$$

Further, according to (5.6),

$$F_1 = F(-ia_1; 1; i\mathbf{p}_1 \cdot \mathbf{r} + i\mathbf{p}_1 \cdot \mathbf{r}),$$

and differentiation of the argument gives

$$\nabla_{\mathbf{r}}(i\mathbf{p}_1 \cdot \mathbf{r} + i\mathbf{p}_1 \cdot \mathbf{r}) = (i\mathbf{p}_1/r) \nabla_{\mathbf{p}_1}(i\mathbf{p}_1 \cdot \mathbf{r} + i\mathbf{p}_1 \cdot \mathbf{r}), \quad (6.8)$$

where

$$\nabla_{\mathbf{p}_1} \equiv (\partial/\partial p_{1x}, \partial/\partial p_{1y}, \partial/\partial p_{1z}), \quad (6.9)$$

and  $F_2$  is independent of  $\mathbf{p}_1$ . Therefore we have

$$\begin{aligned} I_2 &= - (i\mathbf{p}_1/2\epsilon_1) \nabla_{\mathbf{p}_1} \int e^{i\mathbf{q} \cdot \mathbf{r}} F_2^* F_1 d^3 r / r \\ &= - (ia/2a_1) \nabla_{\mathbf{p}_1} I_0 |_{\lambda=0}, \end{aligned} \quad (6.10)$$

in which both  $a_1$  and  $\mathbf{q}$  are to be considered independent of  $\mathbf{p}_1$  when operating with  $\nabla_{\mathbf{p}_1}$ . Similarly, since  $F_2^* = F(ia_2; 1; i\mathbf{p}_2 \cdot \mathbf{r} + i\mathbf{p}_2 \cdot \mathbf{r})$ ,

$$I_3 = (ia/2a_2) \nabla_{\mathbf{p}_2} I_0 |_{\lambda=0}. \quad (6.11)$$

The method used in the evaluation of  $I_0$  (involving contour integration) is due to Dr. A. T. Nordsieck.<sup>26</sup> The authors are indebted to Dr. Nordsieck for his generous communication of the essential steps of this evaluation. By a calculation entirely analogous to that

in the accompanying paper,<sup>26</sup> we obtain

$$I_0 = \frac{2\pi}{\alpha} \left( \frac{\gamma}{\alpha} \right)^{ia_1} \left( \frac{\alpha}{\alpha+\beta} \right)^{ia_2} F(-ia_1, ia_2; 1; x), \quad (6.12)$$

where

$$\alpha = \frac{1}{2}(q^2 + \lambda^2), \quad \beta = \mathbf{p}_2 \cdot \mathbf{q} - i\lambda p_2, \quad (6.13)$$

$$\gamma = \mathbf{p}_1 \cdot \mathbf{q} - i\lambda p_1 + \alpha, \quad \delta = \mathbf{p}_1 \cdot \mathbf{p}_2 - p_1 p_2 + \beta, \quad (6.13)$$

$$x = (\beta\gamma - \alpha\delta)/[\gamma(\alpha+\beta)]. \quad (6.14)$$

For small  $\lambda$ , the three quantities  $\alpha$ ,  $\alpha+\beta$ , and  $\gamma$  are all real; in fact we have

$$\begin{aligned} D_1 &\equiv 2(\alpha+\beta)|_{\lambda=0} = 2\mathbf{q} \cdot \mathbf{p}_2 + q^2 \\ &= (\mathbf{k} - \mathbf{p}_1)^2 - p_2^2 = 2k(\epsilon_1 - p_1 \cos\theta_1); \end{aligned} \quad (6.15)$$

$$\begin{aligned} D_2 &\equiv 2(\gamma)|_{\lambda=0} = 2\mathbf{q} \cdot \mathbf{p}_1 + q^2 \\ &= (\mathbf{k} - \mathbf{p}_2)^2 - p_1^2 = 2k(\epsilon_2 - p_2 \cos\theta_2). \end{aligned}$$

Therefore the two powers with imaginary exponent in (6.12) will be of absolute magnitude unity. The argument of the hypergeometric function,  $x$ , can be shown to be between 0 and 1. For most calculations, it is preferable to consider

$$y \equiv 1 - x = \frac{\alpha(\gamma+\delta)}{\gamma(\alpha+\beta)} \Big|_{\lambda=0} \quad (6.16)$$

Some algebra yields

$$y = q^2 \mu / D_1 D_2, \quad (6.17)$$

where

$$\mu = 2(\gamma+\delta)|_{\lambda=0} = k^2 - (p_1 + p_2)^2 \quad (6.18)$$

is a positive quantity (since  $k = \epsilon_1 + \epsilon_2$ ), independent of angles. It is convenient to introduce the abbreviations:

$$K = 4\pi a (D_2/q^2)^{ia_1} (D_1/q^2)^{-ia_2}, \quad |K| = 4\pi a, \quad (6.19)$$

$$V_{12}(x) = F(-ia_1, ia_2; 1; x), \quad (6.20)$$

$$\begin{aligned} W_{12}(x) &= (a_1 a_2)^{-1} dV_{12}/dx \\ &= F(1-ia_1, 1+ia_2; 2; x). \end{aligned} \quad (6.21)$$

We now differentiate (6.12) as required in (6.7), (6.10), and (6.11). For this purpose,  $\mathbf{q}$  must be kept constant, i.e., (6.15) and (6.18) must not be used until after the differentiation. We note that, for  $\lambda=0$ ,

$$-\mathbf{p}_1 \nabla_{\mathbf{p}_1} \delta = \mathbf{p}_2 \mathbf{p}_1 - \mathbf{p}_1 \mathbf{p}_2 \equiv \mathbf{P}, \quad \nabla_{\mathbf{p}_2} \delta = \mathbf{P}/p_2 + \mathbf{q}. \quad (6.22)$$

We obtain

$$\begin{aligned} I_1 &= 2K \left\{ \frac{V_{12}}{q^2} \left( \frac{\epsilon_2}{D_1} - \frac{\epsilon_1}{D_2} \right) \right. \\ &\quad \left. + \frac{iW_{12}}{D_1 D_2} \left[ a_1 \epsilon_2 \left( \frac{\mu}{D_1} - 1 \right) + a_2 \epsilon_1 \left( \frac{\mu}{D_2} - 1 \right) \right] \right\}, \\ I_2 &= K \left\{ -\frac{V_{12}}{D_2} \frac{\mathbf{q}}{q^2} + ia_2 \frac{W_{12}}{D_1 D_2} \left[ \mathbf{q} \left( \frac{\mu}{D_2} - 1 \right) + \frac{\mathbf{P}}{p_1} \right] \right\}, \\ I_3 &= K \left\{ \frac{V_{12}}{D_1} \frac{\mathbf{q}}{q^2} + ia_1 \frac{W_{12}}{D_1 D_2} \left[ \mathbf{q} \left( \frac{\mu}{D_1} - 1 \right) - \frac{\mathbf{P}}{p_2} \right] \right\}. \end{aligned} \quad (6.23)$$

\* A. T. Nordsieck, following paper in this issue. The integration was already carried out by Bess, but it is somewhat more difficult to follow the complex arguments of all the quantities involved in Bess' paper.

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In the limit of high energies,  $a_1 = a_2 = a$  with an error of the relative order  $1/\epsilon^2$ . We may therefore replace  $V_{12}$  and  $W_{12}$ , respectively, by

$$\begin{aligned} V(x) &= F(-ia, ia; 1; x) \\ &= 1 + \frac{a^2}{1!^2} x + \frac{a^2(1+a^2)}{2!^2} x^2 \\ &\quad + \frac{a^2(1+a^2)(2^2+a^2)}{3!^2} x^3 + \dots, \quad (6.24) \end{aligned}$$

$$\begin{aligned} W(x) &= a^{-2} dV/dx \\ &= 1 + \frac{1+a^2}{1!2!} x + \frac{(1+a^2)(2^2+a^2)}{2!3!} x^2 + \dots. \quad (6.25) \end{aligned}$$

Both of these functions are real so that the expressions for  $I_1$  to  $I_3$ , (6.23), fall into a real part proportional to  $V$  and an imaginary part proportional to  $W$ . The resulting cross section therefore contains only  $V^2$  and  $W^2$ , not  $vw$ .

In the cross section we require the absolute square of the matrix element  $H_{12}'$ , Eq. (5.1), summed over the spin directions of electron and positrons, and averaged over the directions of polarization of the incident quantum. Since the spin sums of  $|H_{12}'|^2$  involve the free-electron Dirac matrix coefficients  $u_1$  and  $u_2$  we may use the spur and closure theorems. From (6.2) we have then

$$\begin{aligned} \Sigma |H_{12}'|^2 &= |C'|^2 (\epsilon_1 \epsilon_2)^{-1} \\ &\times \sum_{\nu=1}^2 \{ I_{1\nu}^2 (\epsilon_1 \epsilon_2 + 1 - p_1 p_2 \cos \theta_1 \cos \theta_2) \\ &\quad + (I_{2\nu}^2 + I_{3\nu}^2) (\epsilon_1 \epsilon_2 - 1 + p_1 p_2 \cos \theta_1 \cos \theta_2) \\ &\quad - 2 I_{2\nu} I_{3\nu} (\epsilon_1 \epsilon_2 - 1 + p_1 \cdot p_2) \\ &\quad + 2(I_{2\nu} - I_{3\nu}) \cdot (p_2 I_{3\nu}, p_1 - p_1 I_{2\nu}, p_2) \\ &\quad + 2I_{3\nu} \cdot p_2 I_{2\nu} \cdot p_1 - 2I_{2\nu} \cdot p_2 I_{3\nu} \cdot p_1 \\ &\quad + 2I_{1\nu} \epsilon_2 (I_{2\nu} \cdot p_1 - I_{3\nu} p_{1z}) \\ &\quad + 2I_{1\nu} \epsilon_1 (I_{3\nu} \cdot p_2 - I_{2\nu} p_{2z}) \\ &\quad + 2(p_1 \cdot p_2 - p_1 p_{2z}) I_{2\nu} I_{3\nu} \}, \quad (6.26) \end{aligned}$$

where  $I_{k\nu}$ , with  $\nu = 1$  and  $2$ , denote the real and imaginary part, respectively, of the integral  $I_k$ ,  $k = 1$  to  $3$  (see remarks following Eq. (6.25)). The subscript  $z$  used in the expression above denotes the  $z$  component of the vector to which it applies, i.e., the component in the direction of  $\mathbf{k}$ .

The results (6.23), (6.26) do not differ greatly from Bess' results (37) and (36). In (6.26), the only difference is that Bess omitted the last line which is in fact not important for small angles  $\theta_1, \theta_2$ . In (6.23),  $I_2$  and  $I_3$  differ from Bess' expression only by the denominators  $p_1$  and  $p_2$  in the last terms which are needed for dimen-

sional reasons.  $I_1$  is much simpler than the corresponding expression of Bess which contains a number of additional terms arising from the incorrect part of his wave function.<sup>21</sup> It is reasonable that the results should differ only in  $I_1$  because Bess' additional term in  $\psi, (a/2\epsilon)\partial F/\partial r$ , involves no matrix operator and should have the same matrix factor as the contribution of  $\psi_a$ . A minor change is in the coefficient  $K$  for which Bess has  $4\pi a(D_1/D_2)^{1/2}$ ; this does not affect the result.

The transition probability per unit time is

$$w = (2\pi/\hbar) \rho_f \Sigma |H_{12}'|^2, \quad (6.27)$$

where  $\Sigma |H_{12}'|^2$  is given by (6.26) and  $\rho_f$  is the density of final states for the two emitted electrons, i.e.,

$$\rho_f = (mc^2)^4 p_1 \epsilon_1 p_2 \epsilon_2 d\Omega_1 d\Omega_2 (2\pi\hbar c)^{-6}, \quad (6.28)$$

where  $d\Omega_1$  and  $d\Omega_2$  are the solid angles.

The differential cross section,  $d\sigma$ , is equal to the transition probability normalized to unit current of the incident particle. Thus we must divide  $w$  by the velocity of the incident quantum,  $c$ , and obtain

$$\begin{aligned} d\sigma &= \frac{(2\pi)^2 (mc^2)^4}{\hbar c (2\pi\hbar c)^6} p_1 p_2 \epsilon_1 \epsilon_2 \Sigma |H_{12}'|^2 d\epsilon_1 \\ &\quad \times \sin \theta_1 d\theta_1 \sin \theta_2 d\theta_2 d\phi, \quad (6.29) \end{aligned}$$

where  $\phi = \phi_1 - \phi_2$  and the integration over  $\phi_2$  has been carried out, yielding a factor  $2\pi$ .

The factor  $|C'|^2$  in  $|H_{12}'|^2$  is given by (6.4) and (4.2) in terms of the normalization factors  $N_1$  and  $N_2$ . The wave function of the negative electron is asymptotically  $\psi_2 = N_2 e^{i\phi_2} u_2 F_2$ . Since the exponential and  $u_2$  are normalized to unity we must examine the asymptotic behavior of  $F_2$  which is

$$F_2 \sim [\Gamma(1+ia_2)]^{-1} e^{-\pi a_2/2} e^{i\phi_2 \log(p_2 r + p_2 \cdot r)}. \quad (6.30)$$

Thus, normalizing  $\psi_2$  to unit amplitude, we have

$$|N_2|^2 = |\Gamma(1+ia_2)|^2 e^{\pi a_2} = \pi a_2 e^{\pi a_2} / \sinh \pi a_2, \quad (6.31)$$

whereas for the positive electron the sign of  $a$  is reversed, yielding

$$|N_1|^2 = \pi a_1 e^{-\pi a_1} / \sinh \pi a_1, \quad (6.32)$$

with positive  $a_1$ .

Substituting (4.2), (6.4), (6.19), (6.31), and (6.32), we have

$$|C' K|^2 = (4\pi a)^2 \left(\frac{\hbar}{mc}\right)^6 \frac{\pi^2 a_1 a_2 e^{\pi(a_1-a_2)}}{\sinh \pi a_1 \sinh \pi a_2}. \quad (6.33)$$

Upon making the approximations  $a_1 \approx a, a_2 \approx a$  [involving errors of  $O(1/\epsilon^2)$ ], this becomes

$$|C' K|^2 = \frac{(2\pi a)^4}{(\sinh \pi a)^2} \left(\frac{\hbar}{mc}\right)^6. \quad (6.34)$$

Substituting (6.23), (6.26), and (6.34) in (6.29), we

have the differential cross-section for pair production:

$$\begin{aligned}
 d\sigma = & - \left( \frac{\pi a}{\sinh \pi a} \right)^2 \frac{q^2}{2\pi} \left( \frac{\hbar}{mc} \right)^2 \frac{e^2}{\hbar c} \frac{p_- p_+}{k^3} d\epsilon_+ \\
 & \times \sin\theta_- \sin\theta_+ d\theta_- d\theta_+ d\phi \\
 & \times \left\{ \frac{V^2(x)}{q^4} \left[ \frac{p_-^2 \sin^2\theta_+ (4\epsilon_+^2 - q^2)}{(\epsilon_- - p_- \cos\theta_-)^2} \right. \right. \\
 & + \frac{p_+^2 \sin^2\theta_+ (4\epsilon_-^2 - q^2)}{(\epsilon_+ - p_+ \cos\theta_+)^2} \\
 & + \frac{(4\epsilon_- \epsilon_+ + q^2 - 2k^2) 2p_- p_+ \sin\theta_- \sin\theta_+ \cos\phi}{(\epsilon_- - p_- \cos\theta_-)(\epsilon_+ - p_+ \cos\theta_+)} \\
 & - \frac{2k^2 (p_-^2 \sin^2\theta_- + p_+^2 \sin^2\theta_+)}{(\epsilon_- - p_- \cos\theta_-)(\epsilon_+ - p_+ \cos\theta_+)} \\
 & + \frac{a^2 [k^2 - (p_- + p_+)^2]^2 W^2(x)}{[4k^2 (\epsilon_- - p_- \cos\theta_-)(\epsilon_+ - p_+ \cos\theta_+)]^2} \\
 & \times \left. \left. \left[ \frac{p_-^2 \sin^2\theta_- (4\epsilon_+^2 - q^2)}{(\epsilon_- - p_- \cos\theta_-)^2} + \frac{p_+^2 \sin^2\theta_+ (4\epsilon_-^2 - q^2)}{(\epsilon_+ - p_+ \cos\theta_+)^2} \right. \right. \right. \\
 & - \frac{(4\epsilon_- \epsilon_+ + q^2 - 2k^2) 2p_- p_+ \sin\theta_- \sin\theta_+ \cos\phi}{(\epsilon_- - p_- \cos\theta_-)(\epsilon_+ - p_+ \cos\theta_+)} \\
 & + \frac{2k^2 (p_-^2 \sin^2\theta_- + p_+^2 \sin^2\theta_+)}{(\epsilon_- - p_- \cos\theta_-)(\epsilon_+ - p_+ \cos\theta_+)} \\
 & \left. \left. \left. - 4k^2 (\epsilon_- \epsilon_+ + p_- p_+ \cos\theta_- \cos\theta_+) \right] \right] \right\}. \quad (6.35)
 \end{aligned}$$

It will be recognized that the first group of terms, those proportional to  $V^2(x)$ , is identical with the Bethe-Heitler cross section except for the factor

$$[V(x)\pi a / \sinh \pi a]^2. \quad (6.36)$$

It can be shown that<sup>37</sup>

$$V(x=1) = \sinh \pi a / \pi a, \quad (6.37)$$

so that the cross section is simply multiplied by

$$[V(x)/V(1)]^2. \quad (6.38)$$

In addition, there is another group of terms proportional to  $W^2(X)$ . These terms have a form very similar to that of the Bethe-Heitler terms, but the deviations from the latter are real, as will be further demonstrated in the next section.

The pair-production cross section (6.35) may be compared with Bess's result (38) for bremsstrahlung. When the translation from one phenomenon to the other is made in the usual way, the main difference is

<sup>37</sup> Davies, Bethe, and Maximon, Eq. (24), this issue [Phys. Rev. 93, 788 (1954)].

that (6.35) does not contain those terms which arise from Bess' spurious terms in  $I_1$ , i.e., all his terms containing  $a^2 V^2$ ,  $a^2 V W$  or  $a^4 W^2$ . In addition, Bess omitted the  $q^2$  terms in the first square bracket, which is not serious. The second bracket has been completely rewritten to make its similarity with the first bracket evident; apart from this, it differs from Bess' appreciably in content.

## VII. SMALL-ANGLE APPROXIMATION

It is well known that the main contribution to the integral cross section for either pair production or bremsstrahlung comes from small angles,  $\theta_1$  and  $\theta_2$  of order  $1/\epsilon$ . Moreover, our whole approximation, i.e., the representation of the electron wave functions by the contributions  $a$  and  $b$ , alone, Eqs. (2.14), (2.15), is only justified for small angles. It is therefore interesting to investigate the behavior of our matrix elements and cross sections in the limit of small angles. This will permit a considerable simplification, and thereby better insight into the orders of magnitude and the structure of the expression. Furthermore, this simplification is an essential first step in the integration of the cross section over angles.<sup>38</sup>

We introduce the vectors  $u$  and  $v$  to denote the components of  $p_1$  and  $p_2$ , respectively, perpendicular to  $k$ . Their magnitudes are

$$u = p_1 \theta_1, \quad v = p_2 \theta_2, \quad (7.1)$$

if we make the approximation  $\sin\theta_1 = \theta_1$ ,  $1 - \cos\theta_1 = \frac{1}{2}\theta_1^2$  which we shall use generally. It is convenient to split  $q$  into the part in the  $z$  direction and the part perpendicular to  $k$  which are, respectively,

$$q_z = (1+u^2)/2\epsilon_1 + (1+v^2)/2\epsilon_2, \quad (7.2)$$

$$\begin{aligned} q_{\perp} &= -(u+v), \\ q_{\perp}^2 &= u^2 + v^2 + 2uv \cos\phi. \end{aligned} \quad (7.3)$$

Here, and in the following, we neglect consistently terms of relative order  $1/\epsilon^2$ . The minimum value of  $q$ , for  $u=v=0$ , is

$$q_{\min} = q_{z \min} \equiv \delta = k - p_1 - p_2 \approx k/2\epsilon_1\epsilon_2. \quad (7.4)$$

If  $u$  and  $v$  are of order 1,  $q$  is of the same order; but  $q_z$  is generally of order  $1/\epsilon$  and  $q$  can be of that order if the vectors  $u$  and  $v$  are nearly equal and opposite.

The quantities introduced in (6.15) to (6.18) are, in our approximation and notation,

$$D_1 = (k/\epsilon_1)(1+u^2), \quad D_2 = (k/\epsilon_2)(1+v^2), \quad (7.5)$$

$$\mu = 2k\delta = k^2/\epsilon_1\epsilon_2, \quad (7.6)$$

$$y = q^2 / [(1+u^2)(1+v^2)]. \quad (7.7)$$

It will be convenient in the following to use the further

<sup>38</sup> We are indebted to Dr. Handel Davies who carried out the angular integration, for some of the calculations reported in this section.

abbreviations:

$$\xi = 1/(1+u^2), \quad \eta = 1/(1+v^2), \quad (7.8)$$

in terms of which (7.5) and (7.7) can easily be rewritten. If  $k$  and  $\epsilon_1, \epsilon_2$  are regarded as of the same order of magnitude (order  $\epsilon$ ), and are large compared with 1, then  $D_1, D_2, \mu, y, u, v, \xi$ , and  $\eta$  are all of order unity.

The vector  $\mathbf{P}$  introduced in (6.22) has the components

$$\mathbf{P}_\perp = \epsilon_2 \mathbf{u} - \epsilon_1 \mathbf{v}, \quad P_z = (\epsilon_1/2\epsilon_2)v^2 - (\epsilon_2/2\epsilon_1)u^2. \quad (7.9)$$

Since  $p$  occurs only with the denominators  $p_1, p_2$  in (6.23), the component  $P_z$  (which is of order 1) gives a negligible contribution compared with either  $P_\perp$  (order  $\epsilon$ ) or the remaining terms in (6.23).

Inserting into (6.23), we obtain

$$\begin{aligned} I_1 &= 2K(\epsilon_1\epsilon_2/k)[q^{-2}(\eta-\xi)V + ia(\xi+\eta-1)W], \\ I_2 &= K(\epsilon_2/k)[-qq^{-2}\eta V + ia(u+\eta q)W], \\ I_3 &= K(\epsilon_1/k)[qq^{-2}\xi V + ia(v+\xi q)W]. \end{aligned} \quad (7.10)$$

These expressions are very much simpler than (6.23). They show clearly that  $I_1$  is of order  $\epsilon$ , while  $I_2$  and  $I_3$  are of order 1. This is to be expected from the definitions (6.3) in which  $I_2, I_3$  have extra denominators  $\epsilon_1, \epsilon_2$ . It can also be shown by the methods of Sec. IX.

The spin sum (6.26) contains many terms which are negligible in the limit of high energies and small angles. Clearly, the factor of  $I_2^2$  inside the braces of (6.26) is of order  $\epsilon^2$ , therefore the complete expression in the braces must be expected to be (and turns out to be) of this order. This means that we should retain coefficients of order 1 multiplying  $I_1^2$ , of order  $\epsilon$  multiplying  $I_1I_2$  or  $I_1I_3$ , and of order  $\epsilon^2$  multiplying  $I_2^2, I_2I_3$ , or  $I_3^2$ ; all lower powers of  $\epsilon$  can be neglected. Doing this, (6.26) becomes after some algebra,

$$\begin{aligned} \Sigma |H_{12}'|^2 &= |C'|^2(\epsilon_1\epsilon_2)^{-1} \sum \{(2\epsilon_1\epsilon_2)^{-1} \\ &\times (k^2 + \epsilon_2^2u^2 + \epsilon_1^2v^2)I_{1,1}^2 \\ &+ 2I_{1,1}(\epsilon_2\mathbf{u} \cdot \mathbf{I}_{2,1} + \epsilon_1\mathbf{v} \cdot \mathbf{I}_{3,1}) \\ &+ 2\epsilon_1\epsilon_2(I_{2,1}^2 + I_{3,1}^2)\}. \end{aligned} \quad (7.11)$$

This can also be written

$$\begin{aligned} \Sigma |H_{12}'|^2 &= |C'|^2 \sum \{(k^2/2\epsilon_1\epsilon_2)I_{1,1}^2 \\ &+ 2(I_{1,1}\mathbf{u}/2\epsilon_1 + \mathbf{I}_{2,1})^2 + 2(I_{1,1}\mathbf{v}/2\epsilon_2 + \mathbf{I}_{3,1})^2\}. \end{aligned} \quad (7.12)$$

The simplification achieved in (7.11), (7.12) is quite remarkable. The result can also be understood directly by evaluating approximately the matrix elements occurring in (6.2), *viz.*,

$$b = (\mathbf{u}_2^* \alpha_\lambda \mathbf{u}_1), \quad c = (\mathbf{u}_2^* \alpha_\lambda \alpha \mathbf{u}_1), \quad (7.13)$$

between an initial state of energy  $-\epsilon_1$ , momentum  $-\mathbf{p}_1$ , and a final state  $\epsilon_2, \mathbf{p}_2$ . Taking the  $\lambda$  component of  $c$ , we obtain the operator  $\alpha_\lambda^2 = 1$  whose matrix element is very nearly 1 if the spins of electron and positron are parallel. There are two possibilities of achieving this, *viz.*, both spins up or both down; hence the factor

of  $I_2^2$  and  $I_3^2$  should be 2, as indeed it is in (7.12). Only the components of  $I_2$  and  $I_3$  perpendicular to  $\mathbf{k}$  can come in because  $\lambda$  is perpendicular to  $\mathbf{k}$ . If the electron and positron have opposite spin, the matrix element of  $c_\lambda$  is of order  $1/\epsilon$ .

The matrix element  $b$ , for parallel spin of electron and positron, represents the sum of the velocities of the two particles in the direction of  $\lambda$  (or, after summing over polarization, the velocity component perpendicular to  $\mathbf{k}$ ). The velocity of the positron perpendicular to  $\mathbf{k}$  (in units of  $c$ ) is  $\mathbf{u}/\epsilon_1$ , that of the electron  $\mathbf{v}/\epsilon_2$ . It is at least plausible that the positron velocity  $\mathbf{u}/\epsilon_1$  will interfere only with  $I_2$  which is due to the correction to the positron wave function, and *vice versa*. The first term in (7.12) arises from the matrix elements of  $b$  which correspond to a reversal of spin.

From (7.12) and from the last two paragraphs, we can see clearly what has already been said in the introduction:  $I_2$  and  $I_3$  have matrix factors of order unity, thanks to the extra operator  $\alpha$  occurring in  $c$ , while  $I_1$  has a matrix factor of order  $1/\epsilon$ . Therefore, even though  $I_1$  itself is much larger than  $I_2$ , *viz.*, of order  $\epsilon$  rather than 1, its contribution to the complete matrix element is only of the same order as that of  $I_2$  or  $I_3$ .

With the simplified expressions (7.10), (7.11), it is now easy to calculate the differential cross section which becomes

$$\begin{aligned} d\sigma &= 8 \left( \frac{\pi a}{\sinh \pi a} \right)^2 \frac{d^2}{2\pi} \left( \frac{\hbar}{mc} \right)^2 \frac{\epsilon^2}{\hbar c} \frac{\epsilon_1^2 \epsilon_2^2}{k^3} d\epsilon_1 d\theta_1 d\theta_2 d\theta_3 d\phi \\ &\times \{q^{-4}V^2(x)[k^2(u^2+v^2)\xi\eta - 2\epsilon_1\epsilon_2(u^2\xi^2+v^2\eta^2) \\ &+ 2(\epsilon_1^2+\epsilon_2^2)uv\xi\eta \cos\phi] + a^2W^2(x)\xi^2\eta^2 \\ &\times [k^2(1-(u^2+v^2)\xi\eta) - 2\epsilon_1\epsilon_2(u^2\xi^2+v^2\eta^2) \\ &- 2(\epsilon_1^2+\epsilon_2^2)uv\xi\eta \cos\phi]\}. \end{aligned} \quad (7.14)$$

This result can also be obtained by making the high-energy, small-angle approximations in (6.35) and taking out a factor  $8\epsilon_1\epsilon_2$  from the braces. However, the fact that (7.14) can also be deduced from the simple theory of this section gives confidence that no algebraic error has been made on its derivation, and that the difference in structure between the factors of  $V^2$  and  $W^2$  is real.

The result (7.14) is also the most suitable starting point for the integration over angles.

### VIII. THE CROSS SECTION FOR BREMSSTRAHLUNG

The matrix element for bremsstrahlung is given in (4.18). Its evaluation is quite similar to that for pair production, with the result, analogous to (6.12),

$$\begin{aligned} I_0 &= \frac{2\pi}{\alpha} e^{-\pi a_1} \left( \frac{\alpha}{\gamma+\delta} \right)^{ia_1} \left( \frac{\gamma+\delta}{\gamma} \right)^{i(a_1-a_2)} \\ &\times F(1-ia_1, ia_2; 1; x), \end{aligned} \quad (8.1)$$

where the meaning of  $\alpha$  and  $\beta$  is the same as in (6.13).

but the other parameters are changed to

$$\gamma = \mathbf{p}_1 \cdot \mathbf{q} + i\lambda p_1 - \alpha, \quad \delta = p_1 p_2 + \mathbf{p}_1 \cdot \mathbf{p}_2 - \beta. \quad (8.2)$$

Also,

$$\mathbf{q} = \mathbf{p}_1 - \mathbf{p}_2 - \mathbf{k}, \quad (8.3)$$

and the argument of  $F$  is

$$x = (\alpha\delta - \beta\gamma) / [\alpha(\gamma + \delta)]. \quad (8.4)$$

It is again more convenient to use

$$y = 1 - x = \gamma(\alpha + \beta) / (\gamma + \delta)\alpha. \quad (8.5)$$

The reason for the appearance of the factor  $e^{-\pi a_1}$  is explained in the paper by Nordsieck following this.

The most important change is that  $\delta$ , Eq. (8.2), now contains the sum of  $p_1 p_2$  and  $\mathbf{p}_1 \cdot \mathbf{p}_2$  rather than their difference, as in (6.13). This change can be traced directly to the form of the matrix element (4.18) for bremsstrahlung which contains  $\mathbf{p}_1 \cdot \mathbf{r}$  and  $\mathbf{p}_2 \cdot \mathbf{r}$  with opposite signs while in the pair matrix elements (5.6) they occur with the same sign. The effect of the changed expression for  $\delta$  is to make this quantity very large, of order  $\epsilon^2$ , if  $\mathbf{p}_1$  and  $\mathbf{p}_2$  have nearly the same direction, as is usual. The three other parameters,  $\alpha$ ,  $\beta$ ,  $\gamma$  in bremsstrahlung, and all four parameters in pair production, are of order 1. Since  $\delta$  is now so large, the definition (6.14) of  $x$  is no longer convenient because it would make  $x$  larger than 1. The changed argument  $x$  in turn causes a change of the first parameter of the hypergeometric function, from  $-ia_1$  to  $1 - ia_1$ . The new definition (8.4) of  $x$  keeps  $x < 1$ ; in fact it is easy to show that  $y = 1 - x$  is in general very small (see below). Since for small angles between  $\mathbf{p}_1$  and  $\mathbf{p}_2$  we may replace  $\delta$  by  $2\epsilon_1\epsilon_2$ , we get

$$y = D_1 D_2 / 4\epsilon_1 \epsilon_2 q^2, \quad (8.6)$$

where  $D_1$  is the same as in (6.15), and

$$\begin{aligned} D_2 = 2(\gamma)_{\lambda=0} &= 2\mathbf{p}_1 \cdot \mathbf{q} - q^2 = p_1^2 - (\mathbf{k} + \mathbf{p}_2)^2 \\ &= 2k(\epsilon_2 - p_2 \cos\sigma_2) \end{aligned} \quad (8.7)$$

is given by the same final expression as in (6.15) even though intermediate steps are different. Since  $D_1$  and  $D_2$  are of order 1,  $y$  will in general be of order  $1/\epsilon^2$  (i.e., where  $q$  is of order 1) but will be larger for small  $q$ . In particular, if both  $\mathbf{p}_1$  and  $\mathbf{p}_2$  are in the direction  $\mathbf{k}$ , then  $q$  attains its minimum value (7.4);  $u$  and  $v$ , Eq. (7.1), are zero and this makes  $y = 1$  and  $x = 0$ . Thus the argument of  $F$  in (8.1) is extremely close to one except for very small  $q$ : this is the essential difference between the results for bremsstrahlung and pair production.

We must now differentiate (8.1) with respect to  $\lambda$ ,  $\mathbf{p}_1$ , and  $\mathbf{p}_2$  as required by (6.7), (6.10), and (6.11). Consider first the differentiation of the factors in front of  $F$ . Of these,  $\alpha$  does not depend on  $\lambda$  in first order, nor on the  $\mathbf{p}$ 's;  $\gamma$  has the exponent  $i(a_1 - a_2)$  which is of order  $1/\epsilon^2$ , and  $\delta$  is so large that  $\partial \log(\gamma + \delta) / \partial \lambda$ , and the other derivatives, are small of order  $1/\epsilon$  or less. Thus one can show that the differentiation of the factors

outside of  $F$  in (8.1) contributes only a term of relative order  $1/\epsilon$  which may be neglected.

It is then only necessary to differentiate with respect to the argument  $x$  of the hypergeometric function, and we obtain

$$I_1 = \frac{2K}{a} \frac{1}{q^2} \frac{dF}{dx} \left( \frac{p_1}{D_2} - \frac{p_2}{D_1} \right), \quad (8.8)$$

where

$$K = 4\pi a e^{-\pi a_1} (q^2 / 4\epsilon_1 \epsilon_2)^{ia_1} (4\epsilon_1 \epsilon_2 / D_2)^{i(a_1 - a_2)}. \quad (8.9)$$

We now transform the hypergeometric function. Setting  $a_1 = a_2 = a$ , it can easily be shown that

$$\begin{aligned} F &\equiv F(1 - ia, ia; 1; x) = F(-ia, ia; 1; x) \\ &\quad + iax F(1 - ia, 1 + ia; 2; x) = V(x) + iax W(x), \end{aligned} \quad (8.10)$$

with  $V$  and  $W$  defined in (6.24), (6.25). One of the terms occurring in (8.8) is then

$$y \frac{d}{dx}(xW) = a^{-2} (1 - x) \frac{d}{dx} \left( x \frac{dV}{dx} \right). \quad (8.11)$$

Now the hypergeometric function  $F(a, b; c; x)$  satisfies the differential equation<sup>39</sup>

$$x(1-x)F'' + [c - (a+b+1)x]F' - abF = 0. \quad (8.12)$$

For  $V = F(-ia, ia; 1; x)$ , this becomes

$$x(1-x)V'' + (1-x)V' - a^2 V = 0, \quad (8.13)$$

and, therefore,

$$(1-x) \frac{d}{dx} \left( x \frac{dV}{dx} \right) = a^2 V. \quad (8.14)$$

Inserting in (8.8), (8.10), (8.11) gives

$$I_1 = 2K q^{-2} (p_2 / D_2 - p_1 / D_1) [V - iayW]. \quad (8.15)$$

This is just the first part  $I_1$  in (6.23), with  $V(x)$  replaced by  $V - iayW$ . Similarly,  $I_2$  and  $I_3$  also become equal to the first term in the respective formulas (6.23), with the same replacement.<sup>40</sup> This result is very similar to the Born approximation which corresponds to taking the limit  $a = 0$ . Doing this in Eq. (6.23) removes the second term which is proportional to  $aW$ , and replaces  $V$  by 1. Thus our result agrees with the Born approximation except for a factor.

To determine this factor, we must consider the normalization factors of the initial and final electron wave function,  $N_1$  and  $N_2$ .  $N_2$  is given by (6.31) and, in our case,  $N_1$  will be given by a similar formula because the initial state is now also an electron of positive energy, whereas the normalization factor (6.32) applied to a negative-energy electron. The two normalization factors  $|N_1 N_2|^2$  together yield a factor  $e^{i(a_1 + a_2)}$ , but our ex-

\* E. T. Whittaker and G. N. Watson, *A Course of Modern Analysis* (The Macmillan Company, New York, 1946), p. 283.

<sup>40</sup> There are also some changes of sign, due to the difference between pair production and bremsstrahlung; these are the same as in Born approximation.

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pression (8.9) shows that  $|C'K|^2$  now contains a factor  $e^{x(a_2-a_1)}$ , just as in (6.33), and for high energies this factor goes to one. This leaves the same factor as compared with the Born approximation as in (6.34), *viz.*,

$$\pi = (\pi a / \sinh \pi a)^2. \quad (8.16)$$

This expression is closely related to the hypergeometric function  $V(x)$  for  $x=1$ . In fact, we have<sup>41</sup> for argument 1:

$$F(a, b, c, 1) = \frac{\Gamma(c)\Gamma(1-a-b)}{\Gamma(1-a)\Gamma(1-b)}, \quad (8.17)$$

and therefore from the definition (6.24)

$$V(1) = \frac{\Gamma^2(1)}{\Gamma(1-ia)\Gamma(1+ia)} = \frac{\sinh \pi a}{\pi a}. \quad (8.18)$$

Therefore, when the normalization factor is included, the matrix element for bremsstrahlung differs from that in Born approximation by the factor

$$[V(x) - iayW(x)]/V(1), \quad (8.19)$$

and the cross section by the factor

$$R = [V^2(x) + a^2y^2W^2(x)]/V^2(1). \quad (8.20)$$

As we have already mentioned after (8.7), the argument  $x$  of the hypergeometric function is almost always very close to one. Whenever this is so, we may use the result of Davies, Bethe, and Maximon, *viz.*, that for  $y=1-x$  near zero,

$$W(x) = -V(1) \log y. \quad (8.21)$$

Then  $yW(x) \sim y \log y$  is very small, and the factor (8.20) becomes equal to unity. Thus, for most of the possible angles,  $\theta_1$ ,  $\theta_2$ , and  $\phi$ , the differential cross section for bremsstrahlung is given exactly by the Born approximation. This is in contrast to the cross section for pair production, and is probably due to the fact that the scattered waves for the initial and final electron do not overlap appreciably in bremsstrahlung (see Sec. IV) while they do for pair production (Sec. V).

An exception is the case of  $q$  very close to its minimum value,  $\delta$ . Then, as shown below Eq. (8.7), the argument  $x$  is substantially below 1, and then  $R$ , Eq. (8.20), will differ from unity. In fact, it can easily be shown to be always less than 1. For this purpose, we take the derivative of the numerator of (8.20) with respect to  $x$  (note  $y=1-x$ ):

$$dR'/dx = VdV/dx - a^2yW^2 + a^2y^2WdW/dx. \quad (8.22)$$

Using (8.14), we find

$$dR'/dx = a^2yWdW/dx. \quad (8.23)$$

But from the power series expansion (6.25) it is clear that both  $W$  and  $dW/dx$  are positive for all  $x$  between

<sup>41</sup> E. T. Whittaker and G. N. Watson, *A Course of Modern Analysis* (The MacMillan Company, New York, 1946), p. 282, reference 39.

0 and 1. Therefore (8.20) increases monotonically with  $x$ , and since it reaches 1 at  $x=1$ , it is less than 1 for any other value of  $x$ .

Thus we have shown that the bremsstrahlung cross section is always less than the Born approximation value. Concerning the integration over angle, there is one limiting case for which the result is obvious, namely that of complete screening: in this limit, the differential cross section for small  $q$  is essentially eliminated by the atom form factor  $F(q)$ . Then  $q$  cannot come close to its lower limit  $\delta$ , which was the only region in which we obtained a deviation from the Born approximation. Therefore, in the limit of complete screening, the Born approximation is valid for bremsstrahlung.

The integration in the absence of screening has been carried out and will appear shortly. For this limit the correction to the Born approximation turns out to be the same as for pair production [see DBM Eq. (35)]. Experimental cross sections, in which screening is incomplete should therefore (for high energies) be less than the Born approximation value. However, the reduction will be less than that for pair production, where the influence of screening is only in the region of small momentum transfer, for which the Coulomb correction is unimportant.

This has consequences for the theory of cascade showers in heavy elements: the cross section for pair production is reduced by about 10 percent (for lead) while that for bremsstrahlung is unchanged. Therefore the ratio of high-energy photons to electrons in the shower is increased by about 10 percent compared with the conventional theory, and the radiation length is increased by about 5 percent.<sup>42</sup>

## IX. THE NEGLIGIBLE MATRIX ELEMENTS

## (a) General

It remains for us to prove that the approximate wave function derived in Secs. II, III is really sufficient for the calculation of the matrix element. In particular, we must consider the correction to the wave function which arises from the term  $a^2/r^3$  in the wave equation, i.e., the function  $\psi_a$  defined by

$$(\nabla^2 + p^2 + 2ea/r)\psi_a = -a^2r^{-2}\psi_a, \quad (9.1)$$

and we must show that its contributions to the matrix element, such as (in the case of bremsstrahlung)

$$I_4 = \int \psi_{2a}^* e^{-ik \cdot r} \psi_{1a} d\tau, \quad (9.2)$$

are actually negligible. It was just this contribution  $I_4$  which Bess tried to take into account, and by which his theory differs from ours. That the contribution from  $I_4$  is negligible will be shown by considering the orders of magnitude of the various contributions to the matrix element.

<sup>42</sup> We are indebted to R. R. Wilson for this remark.

We have discussed orders of magnitude already in Sec. VII. As in that section, we consider  $\epsilon \gg 1$ , and the angles  $\theta_1, \theta_2$  of order  $1/\epsilon$ . Then, as is shown above Eq. (7.9),  $D_1, D_2, \mu, u, v$ , etc., are of order unity. Also  $q$  is in general of this order but it can be as small as  $O(1/\epsilon)$ .

The integral  $I_1$ , involving the main part of the wave function,  $\psi_a$ , is of order  $\epsilon$ , while the integrals  $I_2, I_3$ , involving the correction  $\psi_b$  to the wave function, are of order 1, Eq. (7.10). The matrix factor  $b$ , multiplying  $I_1$ , is of order  $1/\epsilon$ , as shown below (7.13), while the matrix factor  $c$ , multiplying  $I_2$  and  $I_3$ , is of order 1.

Now  $\psi_b$  satisfies the differential equation

$$(\nabla^2 + p^2 + 2ea/r)\psi_b = ia\alpha \cdot \nabla(1/r)\psi_a, \quad (9.3)$$

which is similar to (9.1) in that the right-hand side is of order  $\psi_a/r^2$  in both equations. The order of magnitude of  $\psi_b$  must therefore be expected to be the same as that of  $\psi_a$ , and the order of  $I_4$  the same as  $I_2$  and  $I_3$ , namely unity. In Subsection c, we shall prove this statement in detail; but in Bess's paper  $I_4$  comes out to be of order  $\epsilon$ , like  $I_1$ , which is an unreasonable result.

Now the wave function  $\psi_b$ , like  $\psi_a$ , obviously contains no operators  $\alpha$ , and therefore the integral  $I_4$  will simply be multiplied by the matrix factor  $b$ , Eq. (7.13).<sup>43</sup> In Sec. VII,  $b$  was shown to be of order  $1/\epsilon$ ; therefore, if  $I_4$  is of order 1, its contribution to the matrix element is of order  $1/\epsilon$  and hence negligible.

### (b) The Order of Magnitude of $I_1$ and $I_2$

It is useful to discuss in a simple way the orders of magnitude of the principal integrals  $I_1$  and  $I_2$ . The first purpose is to check the validity of order-of-magnitude arguments which will later (Subsection c) be used to estimate  $I_4$ . Secondly, we shall show that there are no unsuspected cancellations by interference, and finally the arguments will give added insight into the mathematics.

We shall use for the integration variables both polar coordinates  $r, \theta$  and cylindrical coordinates  $z, \rho$ , and use the fact that  $q_s \approx \delta \approx O(1/\epsilon)$ , while  $q_0 \equiv q_1$  is in general of order 1. It can be shown that the main contribution to the integral  $I_1$  comes from regions of space in which the hypergeometric functions  $F$  in the matrix element (5.6) can be replaced by their asymptotic expressions. This is permitted if the arguments of the hypergeometric functions are large compared with 1, viz.,

$$p_1 r + p_1 \cdot r \gg 1. \quad (9.4)$$

Putting the  $z$  axis in the direction of  $-p_1$ , this means

$$p_1(r-z) \approx \frac{1}{2} p_1 r \theta^2 \gg 1, \quad (9.5)$$

or

$$\theta \gg \theta_0 = (p_1 r)^{-1}. \quad (9.6)$$

If  $r \leq \epsilon$ , then  $\theta_0$  as defined by (9.6) is larger than or equal to  $1/\epsilon$ , i.e., to the order of magnitude of  $\theta_1$  and  $\theta_2$ .

<sup>43</sup> In this point, we agree with Bess.

It is then justified, in first approximation, to consider the vectors  $p_1, p_2$  and  $k$  to be essentially in the same direction,  $-z$ .

If the argument  $u_1 = p_1(r-z)$  is large, the hypergeometric function is given by the asymptotic formula

$$F_1 = \frac{e^{ia_1/2}}{\Gamma(1+ia_1)} e^{ia_1 \log u_1} \left( 1 - \frac{ia_1^2}{u_1} \right) - \frac{ie^{ix_1/2}}{\Gamma(-ia_1)} \frac{e^{iu_1 - ia_1 \log u_1}}{u_1} + O\left(\frac{1}{u_1^2}\right). \quad (9.7)$$

Through  $u_1$ , this expression depends on

$$\rho = r\theta; \quad (9.8)$$

we have

$$u_1 = p_1(r-z) \approx p_1 \rho^2 / 2z. \quad (9.9)$$

The other factor depending substantially on  $\rho$  is

$$G \equiv \exp(iq_s \rho). \quad (9.10)$$

It is easy to see that there is no important constructive interference between  $F_1, F_2$ , and  $G$ .

The integral over  $\rho$  arises mainly from values of  $\rho$  up to

$$\rho_1 = 1/q, \quad (9.11)$$

because at larger values of  $\rho$ , rapid oscillations of  $G$  set in. Since the volume element is  $2\pi\rho d\rho dz$  and since the first term of (9.7) does not contain any power of  $\rho$  as a factor, the  $\rho$  integration gives a result of the order

$$1/q^2. \quad (9.12)$$

The integral over  $z$  contains only one important  $z$ -dependent factor, viz.,

$$\exp(iq_s z), \quad (9.13)$$

which shows that values of  $z \approx r$  up to  $1/q$ , contribute, and this quantity is of order  $\epsilon$ . Hence we find from a very simple consideration of orders of magnitude that

$$I_1 \sim \epsilon/q^2, \quad (9.14)$$

which agrees with the explicit evaluation in (7.10).

In  $I_2$  and  $I_3$ , we need the derivative  $dF/du$  which is in the region of validity of the asymptotic expression (9.7):

$$\frac{dF_1}{du} = \frac{1}{u_1} \frac{e^{ia_1 \log u_1}}{\Gamma(ia_1)} \left( \frac{e^{ia_1 \log u_1}}{\Gamma(ia_1)} + \frac{e^{iu_1 - ia_1 \log u_1}}{\Gamma(-ia_1)} \right) + O\left(\frac{1}{u_1^2}\right), \quad (9.15)$$

where the first and second term correspond to the two first terms in (9.7).

We need consider only those components of  $I_2$  and  $I_3$  which have a matrix factor of order unity, i.e., (from (6.2)) are in the  $x$  or  $y$  direction. We have from (6.3a), for example,

$$I_{2x} \sim \frac{1}{\epsilon_1} \int e^{iq_s \cdot r} F_2^* \frac{dF_1}{du_1} (\nabla u_1) d^3r. \quad (9.16)$$

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We use the asymptotic expressions (6.30) and (9.15) for  $F_2^*$  and  $dF_1/du_1$  [from which  $F_2^*$  is essentially of  $O(1)$  and  $dF_1/du_1$  is essentially of  $O(1/u_1)$ , when  $\rho > \rho_0 = r\theta_0 = (r/p_1)^{1/2}$ ],<sup>44</sup> and the small angle approximations (9.9) and

$$(\nabla u_1)_z \approx p_1 \theta \approx p_1 \rho/z, \quad (9.17)$$

[note (9.8)]. The integrals over  $z$  and  $\rho$  are, then, in view of the remark following (9.9),

$$\int \exp(iq_z \rho) d\rho \sim 1/q_z, \quad (9.18)$$

and

$$\int \exp(iq_z z) dz \sim 1/q_z = O(\epsilon), \quad (9.19)$$

so that

$$I_{2z} \sim 1/q_z = O(1), \quad (9.20)$$

in agreement with the explicit result in (7.10).

### (c) The Main Term in the Neglected Part of the Wave Function

In this subsection, we shall discuss the integral  $I_4$ , Eq. (9.2), which arises from the main term in the neglected part of the wave function. We shall show that this is of order 1, i.e., of the same order as  $I_2$ .

We shall evaluate  $I_4$  by replacing  $\psi_{2z}$  by the plane wave,  $e^{ip_2 \cdot r}$ . This amounts to replacing  $N_2 F_2$  by unity, and thus to neglecting some interference effects. The arguments of Subsection b have shown that the elimination of interference effects will not reduce the order of magnitude of the integrals. Furthermore, we take into account that  $N_1$  and  $N_2$  [Eq. (6.31) and remarks preceding Eq. (8.16)] are of order unity.

Then

$$I_4 = \int e^{-i(p_2 + k) \cdot r} \psi_{1z} d^3 r, \quad (9.21)$$

i.e., apart from a constant factor,  $I_4$  is the Fourier component of  $\psi_{1z}$ , corresponding to the momentum  $p_2 + k$ , or it is the momentum-space wave function. To calculate this, we multiply (9.1) on both sides by  $e^{-i(p_2 + k) \cdot r}$  and integrate over space. One of the integrals thus occurring we integrate by parts:

$$\begin{aligned} \int e^{-i(p_2 + k) \cdot r} \nabla^2 \psi_{1z} d^3 r \\ = -(p_2 + k)^2 \int e^{-i(p_2 + k) \cdot r} \psi_{1z} d^3 r. \end{aligned} \quad (9.22)$$

Another integral on the left-hand side, viz.,

$$2e \int e^{-i(p_2 + k) \cdot r} \psi_{1z} d^3 r / r, \quad (9.23)$$

<sup>44</sup> Since the integral in (9.16) converges with  $dF_1/du_1 \sim 1/u_1$ , it will certainly converge in the region  $\rho < \rho_0$  where the asymptotic expression (9.15) is not valid and  $dF_1/du_1$  is of order 1 or less.

we neglect; this is an approximation similar to the replacement of  $\psi_{2z}$  by a plane wave (the error is probably smaller if the Coulomb field is neglected in both  $\psi_1$  and  $\psi_2$ ). Then we get

$$I_4 = -\frac{a^2}{p_1^2 - (p_2 + k)^2} \int e^{i(p_1 - p_2 - k) \cdot r} \frac{d^3 r}{r^2}, \quad (9.24)$$

where we have also replaced  $\psi_{1z}$  by the plane wave  $e^{ip_1 \cdot r}$  on the right-hand side of (9.1).

Now

$$p_1^2 - (p_2 + k)^2 = 2k(\epsilon_2 - p_2 \cos \theta_2) = D_2, \quad (9.25)$$

and is of  $O(1)$ , according to (8.7). Therefore, using the definition of  $q$ , Eq. (8.3), the order of magnitude is

$$I_4 \sim \int e^{iq \cdot r} d^3 r / r^2 \sim 1/q. \quad (9.26)$$

As expected, this is of the same order as  $I_2$ , namely independent of  $\epsilon$ , and has also the same  $q$ -dependence as  $I_2$ . In Bess' calculation, the integral corresponding to  $I_4$  turned out to be of the same order as  $I_1$  which is unreasonable.

Together with the arguments about the matrix factor in Subsection a, this shows that the contribution of  $I_4$  is of order  $1/\epsilon$ , and that therefore  $\psi_1$  can actually be neglected.

### (d) Other Contributions

It is rather evident that the contributions from still higher approximations to the wave function are negligible, and that the same is true of cross terms containing "small parts" of both the initial and final wave function, such as

$$I_5 = \int \psi_{2b}^* e^{-ik \cdot r} \psi_{1b} d^3 r. \quad (9.27)$$

This particular term gives a contribution of order  $\epsilon^{-2} \log \epsilon$  to the matrix element, as shown below.

The significant contribution from  $I_5$  will come from those components with matrix factor of order 1, which result from choosing the  $z$  component of  $\psi_{1b}$  and a component of  $\psi_{2b}^*$  perpendicular to  $z$ , or vice versa. Following the order of magnitude estimation of  $I_{2z}$ , we use the asymptotic expression (9.14) and a similar one for  $dF_2^*/du_2$  and consider

$$I_{5zz} \sim \frac{1}{\epsilon_1 \epsilon_2} \int e^{iq \cdot r} \frac{(\nabla u_1)_z (\nabla u_2)_z}{u_1 u_2} d^3 r. \quad (9.28)$$

Noting that

$$\begin{aligned} (\nabla u_2)_z / u_2 &\approx 1/r, & (\nabla u_1)_z &\approx p_1 \theta, \\ u_1 &\approx p_1 r^2/2, & & \end{aligned} \quad (9.29)$$

and using spherical coordinates, we have

$$I_{5zz} \sim \frac{1}{\epsilon^2} \int e^{iq_z r + i q_1 r \theta \cos \phi} dr d\theta d\phi, \quad (9.30)$$

the azimuthal angle  $\phi$  being measured from the direction of  $\mathbf{q}$ . The integral over  $\phi$  gives  $J_0(q_1 r \theta)$  and that over  $\theta$  is then  $1/q_1 r$  for  $q_1 r \gtrsim O(1)$ , and of  $O(1)$  otherwise. The major contribution to the integral over  $r$  is thus in the region  $1 \leq r \leq 1/q_1$  from which we have

$$\int_1^{1/q_1} (q_1 r)^{-1} \exp(i q_1 r) dr \sim \frac{\log q_1}{q_1} = O(\log \epsilon), \quad (9.31)$$

so that  $I_{5zz}$  is of order

$$\epsilon^{-2} \log \epsilon. \quad (9.32)$$

This shows that  $I_5$  is smaller than  $I_4$  which we previously discussed.

The integrals which arise from higher corrections have their integrands more and more concentrated at small  $r$ . Ultimately, the main contribution to the integrals comes from values of  $r$  of the order of one wavelength, i.e.,  $1/p$ . These integrals will then be of order  $1/\epsilon^3$ . Now it might be possible, with sufficient mathematical skill, to actually calculate the contributions of order  $1/\epsilon$ ,  $\epsilon^{-2} \log \epsilon$  and  $1/\epsilon^2$  to the matrix element by explicit evaluation of some of the integrals we have neglected. But there would be very little hope for the numerous contributions of order  $1/\epsilon^3$ ; these can probably be evaluated only in polar coordinates.

## X. ESTIMATE OF ERROR

In Sec. IX we found that the main term neglected in calculating the matrix element comes from  $I_4$  and is of relative order  $1/\epsilon$ . We believe that there are no cancellations from other neglected terms and that the error is indeed of order  $1/\epsilon$ .

Errors are introduced both in the initial and final state wave function. Since  $\epsilon_2 < \epsilon_1$  for bremsstrahlung, the error in the cross section must be estimated to be of order  $1/\epsilon_2$ . It has long been known that the Bethe-Heitler treatment is wrong near the upper limit of the bremsstrahlung spectrum, and corrections have been proposed by Heitler.<sup>45</sup> Probably this problem could now be solved, either using the wave function of this paper or a method similar to that of Harvey Hall.<sup>12</sup>

No approximation is made in the wave function of the quantum,  $e^{ik \cdot r}$ . Hence the theory is expected to remain correct for small  $k$ .

The total cross section for pair production (or the total energy radiated in bremsstrahlung) is obtained by integration over  $\epsilon_2$ . Since all energies  $\epsilon_2$  between 1 and  $\epsilon_1$  contribute about equally, the relative error in the total cross section is about

$$\Phi = \int_1^{\epsilon_1} \varphi(\epsilon_2) d\epsilon_2 / \epsilon_1, \quad (10.1)$$

where  $\varphi(\epsilon_2)$  is the relative error at  $\epsilon_2$ . Thus, if

$$\varphi \sim 1/\epsilon_2, \quad \Phi \sim \epsilon_1^{-1} \log \epsilon_1. \quad (10.2)$$

For pair production,  $k$  should be substituted for  $\epsilon_1$ .

<sup>45</sup> W. Heitler, *The Quantum Theory of Radiation* (Oxford University Press, London, 1944).

**Masses of Light Atoms from Transmutation Data**  
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The masses of some light atoms, notably  $^9Be$  and  $^{12}C$ , determined by mass spectrograph, did (in 1935) not agree with data from nuclear transmutations. This paper stimulated K. Bainbridge to repeat the mass spectrograph measurements; his results were compatible with nuclear reaction data.

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### Masses of Light Atoms from Transmutation Data\*

The difficulty of reconciling the stability of the Be nucleus with its high mass (9.0154) derived from the mass spectroscopic measurement of Bainbridge is well known. On the other hand, all transmutation data point to a much lower value (about 9.011). If one tries to account for the disintegrations of Be assuming the Bainbridge mass, one is forced to assume the existence of new nuclei, *viz.*,  $\text{Be}^8$  and  $\text{He}^4$ . These present new stability difficulties; e.g., for  $\text{He}^4$  a mass of 5.006 can be derived from transmutation data,<sup>1</sup> which would make  $\text{Li}^6$  unstable against proton emission.

The difficulties are not restricted to Be. Indeed, the energy balance of the disintegration of  $\text{B}^{11}$  under proton bombardment can only be brought into agreement with nuclear masses, by making very artificial assumptions.<sup>2</sup> Other evidence of a wrong determination of the B mass is the transmutation  $\text{B}^{10} + \text{n}^1 = \text{Li}^7 + \text{He}^4$  recently observed by Taylor and Goldhaber.<sup>3</sup>

The most striking instance seems however to be provided by  $\text{C}^{12}$ . The  $\text{C}^{12}$  nucleus is known to emit  $\gamma$ -rays of 5.5 MV,<sup>4, 5, 6</sup> therefore it must have an excited level of this energy which does not disintegrate into 3  $\alpha$ -particles before the  $\gamma$ -ray is emitted. The probability of emission of a  $\gamma$ -ray is about 1 in 10,000 periods of oscillation of the  $\alpha$ -particle in the nucleus. The penetrability of the nuclear barrier for  $\alpha$ -particles must therefore be smaller than 1/10,000 for the excited state, in order that strong  $\gamma$ -radiation can be observed. The energy of the excited state can, then, not be greater than that of 3 $\alpha$ -particles +0.7 MV; and therefore the energy of the ground level must be at least 4.8 MV lower than 3 $\alpha$ 's. Hence

$$\text{C}^{12} < 3 \times 4.00216 - 0.0051 = 12.0014$$

as compared to Aston's value 12.0036.

On the other hand, a lower limit for the mass of  $\text{C}^{12}$  can be obtained from the  $\gamma$ -rays emitted by  $\text{O}^{16}$ , having an energy of 5.4 MV.<sup>5, 6, 7</sup> By the same reasoning as before we conclude that the excited state of the O nucleus could not emit  $\gamma$ -rays in appreciable amount if its energy would exceed that of  $\text{C}^{12} + \text{He}^4$  by more than 1 MV. Therefore the energy of the O ground state must at least be 4.4 MV lower than that of  $\text{C}^{12} + \text{He}^4$ , so that

$$\text{C}^{12} > 16.0000 - 4.0022 + 0.0047 = 12.0025.$$

This "lower" limit is thus seen to be higher than the upper limit derived above. The only possible way out is

to assume that the mass of helium with respect to oxygen is completely wrong.

Such an assumption would immediately explain why all transmutations of the light elements H, He and Li among each other have energy balances fitting beautifully<sup>1</sup> with the mass spectroscopic values whereas for all nuclear processes in which a heavier atom (Be, B) is transformed into light ones the energy balance seems to be completely wrong. Namely, all the light atoms have been compared very accurately to He in Bainbridge's work, whereas the heavier ones have been referred to oxygen.

The change of the ratio He : O seems also to be in accord with the chemical determinations<sup>8</sup> of the atomic weight of H.

Consequently the derivation of atomic weights purely from disintegration data was attempted. Of the transmutations connecting the elements of the "heavier" to those of the "lighter" group the best investigated is the transformation  $\text{B}^{11} + \text{H}^1 = 3 \text{ He}^4$ . Since all considerations involving the upper limit of the  $\alpha$ -particle energy are open to criticism,<sup>9</sup> we have used the mean energy of the emitted  $\alpha$ -particles rather than the maximum energy. This is justified in the case of boron, because it is known<sup>2</sup> that, if  $\gamma$ -rays are emitted at all in the process, there must be less than one  $\gamma$ -ray in 50 disintegrations. Also, there is no other conceivable process which could lead to the emission of low energy particles which could falsify our mean energy: The process  $\text{B}^{10} + \text{H}^1 = 2 \text{ He}^4 + \text{He}^3$  would, even with so high a value for the  $\text{B}^{10}$  mass as 10.0146, set free an energy of only 1 MV, therefore the  $\alpha$ -particles of this process could, even under most favorable conditions, not have more than 4 mm range. On the other hand, in the Wilson chamber measurements of Kirchner<sup>9</sup> which we have used for determining the energy distribution of the  $\alpha$ -rays, no tracks under 5 mm have been measured at all. The latter fact makes incidentally our determination of the energy evolved in the process an upper limit.

The actual calculation gave for the mean energy of the  $\alpha$ -particles observed by Kirchner  $2.85 \pm 0.03$  MV, corresponding to a total energy of all three particles of  $8.55 \pm 0.10$  MV, in perfect agreement with the value deduced from the upper limit of the  $\alpha$ -particle energy (8.7 MV) under the assumption that the fastest  $\alpha$ -particles get just  $\frac{2}{3}$  of the total energy available which follows from momentum considerations.<sup>10</sup> Therefore we consider it as definitely established that the energy evolved in the disintegration of  $\text{B}^{11}$  by proton bombardment is  $8.5 \pm 0.2$  MV, the energy

## LETTERS TO THE EDITOR

of the incident protons being about 150,000 volts in the experiments of Kirchner<sup>9</sup> and of Rutherford and Oliphant.<sup>10</sup> This makes the mass of  $B^{11}=11.0078$ , referred to He = 4.00216.

$B^{10}$  can then be immediately determined from Cockcroft's results<sup>11, 12</sup> on the transmutation  $B^{10}+H^2=B^{11}+H^1$ , which gives  $B^{10}=10.0116$  in agreement with the estimate of Taylor and Goldhaber<sup>3</sup> from the disintegration  $B^{10}+n^1=Li^7+He^4$ .

$C^{12}$  is very well connected with  $B^{10}$  by the reaction  $B^{10}+He^4=C^{12}+H^1$ , investigated by Chadwick<sup>13, 14</sup> and many others.  $C^{12}$  can then be determined from Cockcroft's<sup>11, 12</sup> reaction  $C^{12}+H^2=C^{13}+H^1$ . It is safe to assume that the  $\gamma$ -rays emitted<sup>5</sup> in the process are not connected with the observed proton group of 3 MV, but with another group of such small range that it escapes detection. There are many arguments in favor of this assumption: Firstly, the yield of protons is over 10 times the  $\gamma$ -ray yield.<sup>11</sup> Secondly, if the  $\gamma$ -ray was associated with the 3 MV protons, the stability difficulty for the excited state of the C nucleus pointed out above would not be solved, since the  $C^{12}$  mass would be 12.0030 referred to He (upper limit 12.0014). Thirdly, it has never been observed and is indeed very unlikely from the theoretical point of view, that a transmutation leads *always* to the excited state of the final nucleus, and even 0.2 percent of faster protons would not have escaped detection.<sup>13</sup> Furthermore, the energy of the neutrons from  $\alpha$ -bombardment of Be could not be reconciled with the high C mass 12.0030, and this applies to even greater extent to the neutrons from the reaction  $B^{11}+He^4=N^{14}+n^1$ : Finally, the choice of the lower value of the C mass makes it possible to reconcile our masses with Bainbridge's determination of the Be mass referred to C (see below), and of the  $B^{11}$  mass referred to C and O.

$C^{12}$  being determined, the rest is straightforward:  $N^{14}$  is obtained from Lawrence's data<sup>15</sup> on the process  $N^{14}+H^2=C^{12}+He^4$ , then  $O^{17}$  from Haxel's<sup>16</sup> experiments on  $N^{14}+He^4=O^{17}+H^1$ , and finally  $O^{16}$  from Cockcroft's<sup>11</sup>  $O^{16}+H^2=O^{17}+H^1$ . The result is

$$O^{16}=15.9952, \text{ referred to He}=4.00216.$$

The ratio He : O appears therefore to be wrong by 3.0 parts in 10,000.

Changing back to  $O^{16}=16.17$ , we obtain the following values for the atomic weights of the lighter nuclei:

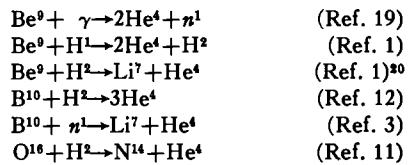
$n^1=1.008\ 5 \pm .000\ 5$	$Be^9=9.013\ 5 \pm .000\ 7$
$H^1=1.008\ 07 \pm .000\ 07$	$B^{10}=10.014\ 6 \pm .001\ 0$
$H^2=2.014\ 23 \pm .000\ 15$	$B^{11}=11.011\ 1 \pm .001\ 1$
$H^3=3.016\ 10 \pm .000\ 33$	$C^{12}=12.003\ 7 \pm .000\ 7$
$He^3=3.016\ 99 \pm .000\ 46$	$C^{13}=13.006\ 9 \pm .000\ 7$
$He^4=4.003\ 36 \pm .000\ 23$	$N^{14}=14.007\ 6 \pm .000\ 4$
$Li^6=6.016\ 14 \pm .000\ 50$	$N^{15}=15.005\ 3 \pm .000\ 5$
$Li^7=7.016\ 94 \pm .000\ 48$	$O^{17}=17.004\ 0 \pm .000\ 2$

referred to  $O^{16}=16.000\ 00$ . The error in the lighter group is mainly due to insufficient knowledge of the ratio He : O, the accuracy of the determinations of the lighter elements with respect to He is much higher.<sup>18</sup>

It is seen that the atomic weights of the heavier group

of elements (Be to O) has only been changed within the limits of error of the mass spectroscopical determinations. This applies even to Be, because this element has been measured with respect to C and  $CH_4$  comparing the ratios Be : C and C :  $CH_4$ . The increase of the atomic weight of H brings Bainbridge's value for Be down to  $9.0145 \pm 0.000\ 6$ , which agrees with our value nearly within the limits of error.

The suggested change of the He : O ratio makes the energy balances for *all* nuclear transformations correct, including those not used in the determination of atomic weights; e.g.



It also explains why no long range  $\alpha$ -particles are observed when  $Be^9$  is bombarded by protons (14): The reaction  $Be^9 + H^1 \rightarrow Li^7 + He^4$  should set only 1.6 MV energy free, of which the  $\alpha$ -particle should receive 1 MV, corresponding to a range of about 5 mm. Particles of this range are observed, but the  $\alpha$ -particles seem to be masked by the longer range (7 mm) deuterons.

The values of the above table are still somewhat uncertain because of the fact that range-energy relation of fast particles is involved. This relation is at present being reconsidered from the theoretical point of view, and there seems to be every hope of reducing the uncertainties due to this factor to a minimum. When these new data are available, it is hoped to make the fourth decimal of the atomic weight significant. The calculations will also be extended to heavier nuclei and, if possible, to some of the artificially radioactive ones. The increased accuracy of atomic weights will also no doubt be helpful in theoretical considerations on nuclear structure.

H. BETHE

Cornell University,  
March 27, 1935.

\* Immediately before this note was sent to press, it came to my knowledge (Science, March 22, 1935) that Oliphant had arrived at essentially the same conclusions as pointed out here. No detailed account of Oliphant's arguments are yet available.

<sup>1</sup> Oliphant, Report London Conference.

<sup>2</sup> Lauritsen and Crane, Phys. Rev. **45**, 493 (1934).

<sup>3</sup> Taylor and Goldhaber, Nature **135**, 341 (1935).

<sup>4</sup> Bothe and Becker, Zeits. f. Physik **76**, 421 (1932).

<sup>5</sup> Crane and Lauritsen, Report London Conference.

<sup>6</sup> Crane, Delsasso, Fowler and Lauritsen, Phys. Rev. **46**, 109 (1934).

<sup>7</sup> MacMillan, Phys. Rev. **46**, 868 (1934).

<sup>8</sup> Aston, *Mass Spectra and Isotopes*, p. 101.

<sup>9</sup> Kirchner, Physik. Zeits. **34**, 897 (1933).

<sup>10</sup> Oliphant and Rutherford, Proc. Roy. Soc. **A141**, 266 (1933).

<sup>11</sup> Cockcroft, Report London Conference.

<sup>12</sup> Cockcroft and Walton, Proc. Roy. Soc. **A144**, 704 (1934).

<sup>13</sup> Chadwick, Constable and Pollard, Proc. Roy. Soc. **A130**, 463 (1931).

<sup>14</sup> Chadwick, Report to the London Conference on Nuclear Physics.

<sup>15</sup> Lawrence, MacMillan and Henderson, Phys. Rev. **47**, 273 (1935).

<sup>16</sup> Haxel, Zeits. f. Physik **93**, 400 (1935).

<sup>17</sup> The question of changing to the scale He = 4.0000 might be reconsidered at this moment when all atomic weights have to be changed anyhow.

<sup>18</sup> It is an advantage of the mass determination by transmutation data that the determination of neighboring elements relative to each other is much more accurate than that of the absolute atomic weight because the relative masses of neighboring elements are needed in predicting the energy evolved in unknown transmutations.

<sup>19</sup> Szillard and Chalmers, Nature **134**, 494 (1934).

<sup>20</sup> This process has been interpreted previously as  $Be^9 + H^2 \rightarrow Li^6 + He^4$ . The assumption of the existence of  $He^4$  is now no longer necessary.

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**The Maximum Energy Obtainable from the Cyclotron**  
(with M. E. Rose)

*Phys. Rev.* **52** (12), 1254–1255 (1937)

This paper caused a lot of controversy. I received many letters from the Berkeley Laboratory, culminating in one from E. O. Lawrence, which contained the sentence “There are many ways to skin a cat.” In 1945, the cat *was* skinned by E. McMillan of Berkeley (and simultaneously by Veksler in the Soviet Union) by inventing the frequency modulated cyclotron whose frequency changes so as to insure focusing. With this, arbitrarily high energies can be and have been obtained.

Other work in the years 1935–37 was summarized in 3 articles in *Rev. Modern Phys.*: **8**, 82–229 (1936); **9**, 69–244 and 245–390 (1937).

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### The Maximum Energy Obtainable from the Cyclotron

It is the purpose of this note to show that a very serious difficulty will arise when the attempt is made to accelerate ions in the cyclotron to higher energies than obtained thus far. This difficulty is due to the relativistic change of mass which has the effect of destroying either resonance or focusing. Since the resonance condition is extremely sensitive, quite small changes of mass, of the order of less than one percent, will have serious effects.

For exact resonance, the magnetic field  $H^0$  must be given by

$$\omega = zeH^0/Mc, \quad (1)$$

where  $\omega$  is the frequency of the electric field and  $ze$  is the charge of the ion.  $M$  is the relativistic mass

$$M = M_0(1+E/M_0c^2), \quad (2)$$

$M_0$  being the rest mass and  $E$  the ion energy. As the energy increases with increasing distance from the source, the resonance field  $H^0$  increases also. At first sight it would seem natural to make the actual field equal to  $H^0$  everywhere. Unfortunately, such a field while maintaining resonance will yield extremely small intensities because practically all the ions will be defocused and thus be lost from the beam (cf. below). Therefore it is necessary to choose a field  $H^1$  which is not exactly the resonance field. At the  $n$ th acceleration the ion will then be off resonance by a phase difference

$$\Delta\theta_n = \pi \int_0^n (H^0/H - 1) dn. \quad (3)$$

Here  $H^0$  and  $H$  are functions of the distance  $r$  from the source,  $r$  being proportional to  $n^2$ . If the phase shift at any point reaches  $\pi$ , an ion which is originally in phase to be accelerated by the electric field, will now be decelerated. Therefore  $\Delta\theta_n$  must always remain very small compared to  $\pi$  (let us say,  $<\pi/6$ ).

Besides the resonance, the most important feature governing the intensity of the emergent beam is the focusing. As will be shown in a subsequent paper,<sup>2</sup> the focusing in the first part of the path is due to the electric field accelerating the ions, and in the second part is due to the magnetic field. The focusing depends on the quantity

$$Q = -\frac{\pi^2}{d \log r} \frac{d \log H}{d \log r} + \pi \frac{\tan \theta}{\nu}, \quad (4)$$

where  $\theta$  is the phase of the electric field at the time of the  $n$ th acceleration of the ion,  $\theta=0$  corresponding to maximum dee voltage. When  $Q$  is positive, focusing of the ions results which is the better the larger  $Q$ . When  $Q$  is negative, the ions are strongly defocused and the beam intensity at the exit slit is reduced by a factor

$$\exp - \int_{r_0}^N |Q(\nu)|^{1/2} d\nu, \quad (5)$$

where  $N$  is the total number of accelerations and  $\nu_0$  is that value of  $\nu$  at which  $Q$  becomes zero.

For large  $\nu$  (large  $r$ ) the first term in (4) (magnetic focusing) will be predominant and must therefore not be negative. This means that, at least for large  $r$ , the magnetic field must not increase with  $r$ . It is just in these regions where an increase is required by the resonance condition (1). Therefore we see that either the resonance or the focusing is destroyed by the relativistic change of mass irrespective of the special choice of the magnetic field.

It is interesting to estimate quantitatively the effects concerned. First we shall assume that the magnetic field is chosen equal to the resonance field. Assuming that  $\nu_0$  (cf. (5)) is small compared to  $N$  which is true for high energies (see below), we find for the beam intensity

$$\exp [-(2\pi N/3)(2E_0/M_0c^2)^{1/2}] = \exp [-2^{1/2}(\pi/3)E_0^{1/2}(M_0c^2)^{-1/2}(Vz)^{-1}], \quad (6)$$

where  $V$  is the accelerating potential and  $E_0$  the final energy of the ion. For protons of 20 MV and  $V=100$  kv, this gives  $e^{-80}$ .

If we want to avoid this magnetic defocusing and at the same time preserve exact resonance, we must therefore make the critical  $\nu_0$  at least equal to  $N$ . For a phase  $\theta=45^\circ$ , this gives for the maximum energy obtainable

$$E_m = (M_0c^2 V z / 2\pi)^{1/2}. \quad (7)$$

Somewhat higher energies may, of course, be obtained by sacrificing exact resonance. In order to obtain best results, very careful design of the magnetic field is necessary. In the outer regions ( $\nu >$  about  $\nu_0$ ), the magnetic field should be homogeneous or, perhaps, even decrease slowly. In the inner regions, a moderate increase is permissible. At the boundary of the two regions ( $\nu \sim \nu_0$ ) the field should be slightly too large for resonance so that the ions will, in the outer region, first gain phase compared to the electric field and will only afterwards start losing phase. If we consider a loss of phase  $\Delta\theta_N \sim \pi/6$  permissible, it will be possible to reach energies roughly twice as high as  $E_m$  (cf. (7)). With a dee voltage of 50 kv, this would permit the production of protons of about 5.5 MV, deuterons of 8 MV and  $\alpha$ -particles of 16 MV. It will be noticed that these limits are very close to the highest energies actually obtained at present. Thus it appears that the cyclotron cannot be made to give much higher energies than those obtained thus far.

The only way to obtain higher energies seems to be to increase the voltage on the dees. But even this will increase the energy limit only moderately, i.e. just as the square root of the dee voltage. Therefore it seems useless to build cyclotrons of larger proportions than the existing ones. With a magnetic field of 18,000 gauss, an accelerating chamber of 37 cm radius will suffice to produce deuterons of 11 MV energy which is the highest obtainable with as much as 100 kv dee voltage. Pole pieces of 34" diameter will be ample for such an accelerating chamber. For a field of 15,000 gauss which has some advantage for the calculation of the necessary "shimming," poles of 40" diameter will be sufficient.

*Note added December 4:* We have found it possible to devise a magnetic field which gives, at 50 kv dee voltage, 12 MV protons, 17 MV deuterons or 34 MV  $\alpha$ -particles with small but measurable intensities. These energies we believe to be the maximum obtainable. A homogeneous field, 0.6 percent greater than the resonance field at the center, will give protons of 10.5 MV, deuterons of 15 MV and  $\alpha$ -particles of 30 MV with somewhat greater intensity.

H. A. BETHE  
Cornell University,  
Ithaca, New York,  
November 24, 1937.

M. E. ROSE

<sup>1</sup>  $H$  denotes the vertical component of the magnetic field.

<sup>2</sup> M. E. Rose, Phys. Rev., to appear shortly.

**Deviations from Thermal Equilibrium in Shock Waves**  
(with E. Teller)  
(1941)

After the fall of France to the Nazis in June 1940, Teller and I felt that we wanted to contribute to the Allied War Effort. Theodor von Karman, the famous aerodynamicist at the California Institute of Technology, was a friend of the Teller family, so we decided to visit him and ask his advice. He suggested the subject. Teller, having worked on molecular physics, knew that approach of the vibrational degree of freedom to thermal equilibrium would be slow, dissociation of the molecule even slower.

This paper has been used widely to guide and interpret experiments. Especially Arthur Kantrowitz and his collaborators have done extensive experiments on shock tubes and, from the behavior of the shock, have deduced rates of excitation of molecular vibrations, of dissociation and of certain chemical reactions, like  $N_2 + O_2 \rightarrow 2NO$ .

DEVIATIONS FROM THERMAL EQUILIBRIUM IN SHOCK WAVES

By

H. A. BETHE

E. TELLER

NOTE

This paper was written by Professor H. A. Bethe of Cornell University and Professor E. Teller of George Washington University before they had any official connections with Government agencies during World War II. Because of the importance of the paper, the Ballistic Research Laboratories, Aberdeen Proving Ground, Aberdeen, Maryland, undertook the reproduction of this paper for limited distribution. This was done with the permission of the authors.

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Deviations from Thermal Equilibrium in Shock Waves

Report by H. A. Bethe, Cornell University, Ithaca, N.Y. in collaboration  
with (sections 1 and 2)  
E. Teller, George Washington University, Washington, D.C.

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## DEVIATIONS FROM THERMAL EQUILIBRIUM IN SHOCK WAVES

## SUMMARY

The various terms contributing to the energy content of a gas, viz. translation, rotation, vibration, electronic excitation and dissociation, are discussed (par. 1). Tables are given of the energy content and the specific heat of a simple harmonic oscillator (Table I), of the energy content and the dissociation of nitrogen, oxygen (Table II) and air (Table III). The molecular vibration becomes important for air at about 600°K, the dissociation at about 3000°K.

The theory of shock waves is generalized to the case when the specific heat changes with temperature (par. 3). General formulae are obtained for the velocity, (3.10), density (3.8a), pressure (3.8b), and temperature (3.9) on the high pressure side. It is shown that the asymptotic values of  $v$ ,  $\rho$ ,  $p$  and  $T$  on the high pressure side at sufficient distance from the front of the shock wave are uniquely determined by the values of these quantities on the low pressure side, and are independent of any intervening phenomena connected with the approach of statistical equilibrium between the various degrees of freedom of the molecule. This we consider the most important result of the present investigations.

A table is given (Table VIII) of the asymptotic values of  $v$ ,  $\rho$ ,  $p$  and  $T$  on the high pressure side as a function of the velocity  $v$  of the shock

wave. The four quantities are calculated (a) using the actual specific heat of air as a function of temperature, as given by Table III (quantities are subscript in Table VIII), and (b) using a constant specific heat equal to that at 300°K (subscript 2). Large differences are found for the temperature in the two calculations ( $T_2 = 8000^\circ$  when  $T_3 = 5000^\circ$ ) and for the density ( $\rho_2 = 5.8$ ,  $\rho_3 = 9.1$ ) but the pressure, which is the most important quantity for applications, is almost independent of the specific heat ( $p_2 = 155$ ,  $p_3 = 168$  atmospheres in the example quoted).

The sudden change of the temperature of a gas when passing through a shock wave destroys temporarily the statistical equilibrium between the various forms of energy of the gas molecules. The degrees of freedom of a molecule can conveniently be divided into two classes, the active ones and the inert ones (par. 2). The "active" degrees of freedom are translation and rotation; they come into thermal equilibrium after one or a few collisions (par. 2A). The most important "inert" degree of freedom is the vibration (par. 2B). Experiments on the absorption of sound show that between 20 and more than 500,000 collisions are necessary to establish thermal equilibrium between vibrations and the active degrees of freedom at room temperature (Table V). This result agrees with the expectation from the theory of Landau and Teller. This theory allows one to predict with moderate accuracy the temperature dependence of  $Z$ , the number of collisions necessary to de-excite the first vibrational quantum state, when a measurement of  $Z$  at one temperature is available (Table IV). Unfortunately no accurate measurements have been made for oxygen and none at all for nitrogen, which makes quantitative statements almost impossible. Therefore we have only listed (Table VI) the values of the mean free path for vibration,  $\lambda_v$  which follow from various assumption (par. 2D) about the efficiency of the collisions. The resulting values of  $\lambda_v$  for the cases which have practical importance for shock waves lie between 3 and 0.0016 millimeters, depending on the vibrating

molecule ( $N_2$  or  $O_2$ ), the assumption made about the efficiency of various molecular collisions, and the humidity of the air.

The dissociation also requires a considerable time to come into equilibrium. The theory (par. 2C) is somewhat more definite in this case than for the vibrations because it depends on the Boltzmann factor rather than on assumptions about the kinetics of collisions. Very large values (from 1 millimeter to 1 meter) are obtained (par. 2D, Table VII) for the mean free path for dissociation,  $\lambda_d$ , in practical cases.

The theory of par. 2 is applied to shock wave in par. 4. It is shown that the shock wave has a sharp front on the low pressure side while on the high pressure side it extends over a distance of the order of the mean free path for vibration,  $\lambda_v$ , or for dissociation,  $\lambda_d$ . Immediately at the wave front, but on the high pressure side, the physical quantities  $P$ ,  $\rho$ ,  $T$ ,  $v$  can be calculated assuming that only the active degrees of freedom exist (Table VIII, quantities with subscripts 2). Going away from the wave front into the high pressure region, the energy  $E_i$  of the inert degrees of freedom increases gradually and approaches the value corresponding to thermal equilibrium. In simple cases,  $E_i$ ,  $p$ ,  $\rho$ ,  $T$  and  $v$  will follow an exponential law (cf. 4.10, 11). If the shock wave is violent enough so that dissociation occurs on the high pressure side, there is first a region of extension  $\lambda_v$  near the wave front in which vibrational equilibrium is established but in which the dissociation is hardly affected, and then a much more extended region (extension  $\lambda_d$ ) in which dissociation takes place.

Two special cases of very soft shock waves are discussed in pars. 5 and 6, these discussions having mostly academic interest. In par. 5, we consider the case where the velocity of the shock wave  $v_1$  is between the actual velocity of sound  $a_1$  and the sound velocity obtained by considering only the active degrees of freedom, i.e.,

$$a_1 < v_1 < a_1 \left(1 + \frac{(c_v - c_{va})R}{2c_v c_{va}}\right) \quad (A)$$

where  $c_v$  is the total specific heat at constant volume and  $c_{va}$  the specific heat due to the active degrees of freedom only. It is shown that in this narrow velocity interval the shock wave is diffuse on the low pressure as well as on the high pressure side. These diffuse shock waves go over automatically into shock waves with a sharp front when  $v_1$  approaches the upper limit given in (A).

In par. 6, slightly faster shock waves are considered, viz. waves for which

$$a_1 \left(1 + \frac{(c_v - c_{va})R}{2c_v c_{va}}\right) < v_1 < a_1 \left(1 + \frac{R}{2c_v + R}\right) \quad (B)$$

For such waves, the temperature on the high pressure side increases with increasing distance from the wave front while for waves of higher velocity  $v_1$ , the temperature has its maximum immediately at the wave front and decreases from there.

NOTATION

Throughout this Report, the following notations will be used:

- $\rho$  = density of gas
- $p$  = pressure (in atmospheres)
- $T$  = temperature in degrees Kelvin
- $E$  = energy content of one gram of gas
- $\alpha$  = degree of dissociation,  

$$1 + \alpha = p / (\rho RT)$$
- $\beta$  =  $\frac{E}{p/\rho} + 1$
- $c_p$  = specific heat at constant pressure per gram
- $c_v$  = specific heat at constant volume per gram
- $\gamma$  =  $c_p/c_v$
- $R$  = gas constant per gram
- $R_o$  = gas constant per mol
- $k$  = Boltzmann's constant (gas constant per molecule)
- $h$  = Planck's constant
- $v$  = velocity of the gas
- $m$  =  $\rho v$  = flow in grams per  $\text{cm}^2$  per sec
- $V$  =  $v + \frac{p}{m}$
- $c$  = velocity which the gas would have if streaming into vacuum
- $a$  = velocity of sound
- $\lambda_v$  = mean free path for vibrations
- $\lambda_d$  = mean free path for dissociation
- $\nu$  = frequency of molecular vibrations
- $D$  = dissociation energy of molecules

SUBSCRIPTS

- a for active degrees of freedom
- i for inert degrees of freedom
- v for vibration
- d for dissociation
- h for an arbitrary point on the high pressure side of a shock wave
- $\lambda$  for an arbitrary point on the low pressure side
- 1 for a point on the low pressure side where thermal equilibrium exists between all degrees of freedom of the molecules
- 2 for a point on the high pressure side immediately at the front of the shock wave
- 3 for a point on the high pressure side at sufficient distance from the wave front so that thermal equilibrium exists

### Par. 1. The Energy Content of Gases

Perfect gases obey the equation of state

$$\frac{p}{\rho} = RT \quad (1.1)$$

where  $p$ ,  $\rho$ ,  $T$  are pressure, density and absolute temperature and where the gas constant  $R$  is a characteristic of the gas considered. If the gas dissociates, (1.1) ceases to be valid; in the particular case of a diatomic gas dissociating into atoms, we have instead:

$$\frac{p}{\rho} = RT(1 + \alpha) \quad (1.2)$$

where  $\alpha$  is the degree of dissociation, i.e., the fraction of molecules dissociated. Generally,  $p/\rho T$  is proportional to the number of separate particles (molecules or atoms) per gram of the substance.

The energy content of a gas consists of five main parts, viz:

- (1) the kinetic energy of the translation of the molecules
- (2) the energy of molecular rotation
- (3) the energy of vibration
- (4) the energy of electronic excitation of the molecule
- (5) the energy of dissociation into atoms (or smaller groups of atoms).

We shall write the total energy content per gram in the form

$$E = (\beta - 1) \left(\frac{p}{\rho}\right) \quad (1.3)$$

The inclusion of the term  $-1$  is convenient because the quantity occurring in the theory of shock waves is  $E + p/\rho$ , where  $p/\rho$  is connected with the work done by the pressure. Furthermore, we shall denote by  $\beta_t$ ,  $\beta_r$ ,  $\beta_v$ ,  $\beta_e$ ,  $\beta_d$  the energy of translation, rotation, vibration, excitation, and dissociation, each divided by  $p/\rho$ , so that

$$\beta = \beta_t + \beta_r + \beta_v + \beta_e + \beta_d + 1 \quad (1.4)$$

The various contributions will now be discussed in order:

1. The translational energy is  $3/2 p/v$  for any gas, independent of the number of atoms per molecule, the temperature, etc.
2. The rotational energy, for all gases except  $H_2$ , and at all temperatures at which the substance is gaseous, is given by the classical kinetic theory of gases without any important quantum correction. It is zero for atoms,  $1 RT$  per gram for diatomic molecules and all polyatomic ones whose atoms lie on a straight line such as  $CO_2$ , and  $3/2 RT$  for all other polyatomic molecules. At high temperatures, there is a correction because the molecules change their shape due to their vibrations. This correction, commonly called the interaction of vibrations and rotations, is usually not very great.
3. The vibrational energy can be approximated (at not too high temperatures) by resolving the vibration into normal modes and treating each mode as a harmonic oscillator.

The number of normal modes is 1 for a diatomic molecules,  $3n-5$  for a molecule containing  $n$  atoms on a straight line and  $3n-6$  for a molecule with  $n$  atoms not on a straight line. The energy contained in one mode is (per gram)

$$E_v = RT \frac{z}{ez - 1} \quad (1.5)$$

where

$$z = \frac{h\nu}{kT} , \quad (1.5a)$$

$\nu$  is the frequency of the vibration,  $h$  Planck's and  $k$  Boltzmann's constant.

If  $\nu$  is given in wave numbers ( $cm^{-1}$ ) and  $T$  in degrees Kelvin,

$$z = 1.438 \nu/T \quad (1.5b)$$

The frequencies of the various normal modes of molecules can be obtained from band spectra. A good survey of data can be found in H. Spener, *Molekülspektren I* (Springer 1935). The frequencies of simple light molecules are very high, e.g. for  $N_2$  we have  $\nu = 2345 \text{ cm}^{-1}$ , for  $O_2$ ,  $1570 \text{ cm}^{-1}$ . For more complicated, and especially for polyatomic molecules, the lowest frequencies are much smaller, the highest ones of the same order as for diatomic ones. E.g.,  $CO_2$  has four modes of vibration with frequencies  $\nu = 667, 667, 1336$  and  $2350 \text{ cm}^{-1}$ .

For low temperatures ( $z$  large), the vibrational energy is negligible. E.g., for  $z = 5$ , it amounts only to  $0.034 RT$ , i.e. 1 per cent of the value of  $E + p/\rho$  for translation and rotation of a diatomic molecule.  $z = 5$  corresponds to  $680^\circ K$  for  $N_2$ ,  $450^\circ$  for  $O_2$  but only  $192^\circ$  for the low frequency mode of  $CO_2$ . Thus the vibrations may be neglected at room temperature for  $N_2$  and  $O_2$  but not for  $CO_2$ .

At high temperatures ( $z$  small), the vibrational energy is  $RT$  per mode. This value is attained very slowly.

TABLE I

## Energy Content of Harmonic Oscillator

$\frac{1}{z} = \frac{kT}{h\nu}$	$\frac{E_V}{RT}$	$\frac{c_V}{R}$	$\gamma$
0.05	$4.1 \cdot 10^{-8}$	$8.2 \cdot 10^{-7}$	1.400
0.1	$4.5 \cdot 10^{-4}$	$4.5 \cdot 10^{-3}$	1.399 <sub>5</sub>
0.15	0.0085	0.0566	1.391
0.2	0.0339	0.170 <sub>5</sub>	1.375
0.25	0.0747	0.304	1.357
0.3	0.123	0.426	1.342
0.4	0.223	0.609	1.321 <sub>5</sub>
0.5	0.313	0.723	1.310 <sub>5</sub>
0.6	0.389	0.800	1.303
0.8	0.502	0.880	1.296
1.0	0.582	0.921	1.292 <sub>5</sub>
1.5	0.704	0.963	1.289
2	0.771	0.979	1.287 <sub>5</sub>
large	$1 - \frac{1}{2} z + \frac{1}{12} z^2$	$1 - \frac{1}{12} z^2$	1.2857

In Table I, we give the vibrational energy of a harmonic oscillator as a function of the temperature. We also give the contribution of the vibration to the specific heat, viz.

$$c_{v,v} = \frac{DE_v}{dT} \quad (1.6)$$

which is seen to become appreciable at much smaller temperatures than  $E_v$ , and to approach its asymptotic value much faster. We have also included the ratio,  $\gamma$  of the specific heats at constant pressure and volume, for a diatomic gas with harmonic oscillation, viz.

$$\gamma = \frac{7/2 R + c_{v,v}}{5/2 R + c_{v,v}} \quad (1.6a)$$

At high temperatures, the vibrations can no longer be regarded as harmonic. The effect of the anharmonicity is to increase the energy content of the gas. E.g., for  $N_2$  at 5000°K the harmonic oscillator model would give  $\beta_v = 0.699$  while the correct value is 0.753, including the interaction of vibration and rotation, and a small contribution from excitation. The influence of the anharmonicity is greater for molecules which are easily dissociated.

4. The electronic excitation is usually rather unimportant compared with vibration and dissociation.

5. The dissociation becomes important at temperatures above 2-3000°K. If  $\alpha$  is the degree of dissociation,  $p$  the total pressure,  $p_A$  and  $p_M$  the partial pressures of atoms and (diatomic) molecules, we have

$$\frac{p_A^2}{p_M} = \frac{4\alpha^2 p}{1-\alpha^2} = K = e^{\Delta F/R_o T} \quad (1.7)*$$

\*  $p$  in (1.7) is considered a dimensionless quantity, viz. the ratio of the pressure to one atmosphere.

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The first equality follows from  $P_A = \frac{2\alpha}{1+\alpha} P$ ,  $P_M = \frac{1-\alpha}{1+\alpha} P$ .  $K$  is the dissociation constant,  $R_o$  the gas constant per mole = 1.987 calories/degree,  $\Delta F = F_M - F_A$  the difference of the free energies per mol of the molecular and the atomic gas, each taken at unit pressure. For some gases, like  $N_2$  and  $O_2$ , tables of  $\Delta F$  as a function of temperature have been published (cf. below). Where they are not published,  $\Delta F$  can be calculated from the Stern-Tetrode formula, which reads for diatomic gases

$$K = \frac{(2\pi m_A k T)^{3/2}}{n h^3} \cdot \frac{g_A^2}{G_M} e^{-\frac{D}{R_o T}} \quad (1.8)$$

where  $m_A$  is the mass of one atom,  $n$  the number of separate particles per  $\text{cm}^3$  of the gas at unit pressure and temperature  $T$ , and  $D$  the dissociation energy in calories per mol. According to spectroscopic evidence (Sponer),  $D$  has the value 117,200 cal. for oxygen and 182,000 cal. for nitrogen, so that  $D/R_o = 59,000$  and 91,600 degrees, respectively.

$g_A$  and  $G_M$  are the statistical weights of the atom and the molecule. In general,  $g_A$  may be put equal to the combined weight of all states of the multiplet to which the ground state belongs, so that

$$g_A = (2L + 1) (2S + 1) \quad (1.9)$$

where  $L$  and  $S$  are orbital angular momentum and spin of the atomic ground state.  $N$ , having a  ${}^4S$  ground state, has therefore  $g_A = (1)(4) = 4$ ; oxygen, with a  ${}^3P$  state, has a weight  $g_A = (3)(3) = 9$ .  $G_M$  consists of three factors referring to the electronic state ( $g_M$ ) of the molecule, the vibration ( $g_v$ ) and the rotation ( $g_r$ ) respectively,

$$G_M = g_M g_v g_r \quad (1.10)$$

$g_M$  can be calculated from spin  $S$  and orbital momentum  $A$ , viz.

$$\begin{aligned} g_M &= 2S + 1 & \text{for } \sum \text{ states } (A = 0) \\ &2(2S + 1) & \text{for all other states } (A \neq 0) \end{aligned} \quad (1.11)$$

The ground state of  $N_2$  is a  $^1\Sigma$  state ( $g_M = 1$ ), that of  $O_2$  a  $^3\Sigma$  state ( $g_M = 3$ ).  $g_r$  is always given with sufficient approximation by classical kinetic theory

$$g_r = \frac{kT}{hB_r} \quad (1.12)$$

where  $B_r$  is defined by the fact that the rotation levels of the molecule are  $B_r j(j+1)$  if  $j$  is the rotational quantum number;  $B_r = 1.44 \text{ cm}^{-1}$  for  $O_2$  and  $2.00 \text{ cm}^{-1}$  for  $N_2$ . If  $B_r$  is measured in  $\text{cm}^{-1}$  and  $T$  in degrees Kelvin,  $g_r = T/1.438 B_r$ . The vibrational part,  $g_v$ , is given by

$$g_v = \frac{1}{1-e^{-z}} \quad (1.13)$$

with  $z$  defined as in (1.5a). Ordinarily, dissociation is only important at high temperatures; then  $g_v$  is sufficiently nearly

$$g_v = kT/h\nu \quad (1.13a)$$

If there are several modes of vibration, there is one factor of the type (1.13) for each mode.

When  $K$  has been calculated, and the total pressure  $p$  is known,  $\alpha$  can be calculated immediately from (1.7), viz.

$$\alpha = \sqrt{\frac{K}{K + 4p}} \quad (1.14)$$

In the theory of shock waves, the density  $\rho$  on the high pressure side can be more readily estimated than the pressure (par. 3). Then, inserting (1.2) in (1.7), we have

$$4RT \rho \alpha^2 (1 + \alpha) = K(1 - \alpha^2) \quad (1.14a)$$

which gives

$$\alpha = -\frac{1}{2} K' + \sqrt{K' + \frac{1}{4} K'^2} \quad (1.15)$$

with

$$K' = \frac{K}{4RT \rho} \quad (1.15a)$$

If  $\rho_0$  is the density of the gas at temperature  $T_0$  and unit pressure, we have

$$K' = \frac{K}{4} \frac{T_0}{T} \frac{\rho_0}{\rho} \quad (1.15b)$$

The dissociation  $\alpha$  depends strongly on the temperature (increasing with increasing  $T$ ) and slightly on the pressure or density (decreasing with increasing  $p$  or  $\rho$ ). The equation of state for a dissociated gas has already been given in (1.2). The energy content is given by

$$\beta = \frac{1 - \alpha}{1 + \alpha} \beta_M + \frac{\alpha}{1 + \alpha} \left( \frac{D}{R_0 T} + 2\beta_A \right) \quad (1.16)$$

where  $\beta_M$  and  $\beta_A$  are the coefficients of energy content for the molecular and the atomic gas at the given temperature. Disregarding the term  $D/R_0 T$ , (1.16) is simply the weighted average of  $\beta_M$  and  $\beta_A$ , the weights being given by the partial pressures. The dissociation itself contributes an energy  $\alpha D$  per mol of the gas; to obtain  $\beta$ , the energy per mol must be divided by  $M_p/\rho = (1 + \alpha)R_0 T$  ( $M$  the molecular weight).

$\beta_M$  can be calculated by adding the contributions 1 to 4 discussed above.  $\beta_A$  is essentially due to translational energy only, and has therefore the value  $5/2$ . (The energy of electronic excitation of the atoms is seldom important below  $5,000^\circ$  and has therefore been neglected.)

At extremely high temperatures (above 5,000°) the ionization of atoms and molecules must be considered. This can be done using similar calculations as for dissociation.

#### Tables

Table II gives the energy constant  $\beta$  of nitrogen and oxygen at temperatures from 300 to 5000° Kelvin. The energy constant from 300° down to the liquefaction temperature remains almost unchanged. The data for nitrogen were taken from W. F. Giauque and J. O. Clayton, Journ. Am. Chem. Soc. 55, 4875 (1933), those for oxygen from H. J. Johnston and M. K. Walker, ibid. 55, 172 (1933). Both sets of data were calculated by the respective authors taking into account all corrections such as anharmonicity of the vibrations, interaction between rotation and vibration, and electronic excitation. The figures given in our table for nitrogen are less accurate because Giauque and Clayton give only the free energy from which the energy content had to be obtained by numerical differentiation, involving considerable inaccuracy. A graphical method was used to smooth out the results of the numerical differentiation. The energy content of  $O_2$  could be read directly from the tables of Johnston and Walker as the difference between  $T$  times the entropy, and the free energy.

The dissociation was calculated for oxygen and nitrogen in air of a density equal to 8 times the density at 300°K and one atmosphere pressure. These conditions were chosen because in a shock wave in which the temperature is raised to 3000-5000°, the density is increased about 8 fold (cf. 3, Table VIII). Obviously, the figures for oxygen would also be valid for pure oxygen of a density of  $(8)(0.210) = 1.680$  times that at 300° and one atmosphere, and the dissociation of nitrogen would be the same for pure nitrogen of a density of  $(8)(0.780_5) = 6.244$  times the density of nitrogen at 300°K and one atmosphere.

Table II. Energy Content and Dissociation of Nitrogen and Oxygen

T	Nitrogen			Oxygen		
	$\beta_M$	K	$\alpha$	$\beta$	$\beta_M$	K
300	3.493			3.493	3.493	
400	3.499			3.499	3.520	
500	3.508			3.508	3.548	
600	3.521			3.521	3.590	
700	3.541			3.541	3.636	
800	3.564			3.564	3.684	
900	3.594			3.594	3.731	
1000	3.625			3.625	3.774	
1250	3.702			3.702	3.871	
1500	3.780			3.780	3.950	
1750	3.845			3.845	4.015	
2000	3.900	$4.0 \cdot 10^{-14}$	$1.55 \cdot 10^{-8}$	3.900	4.068	$5.15 \cdot 10^{-7}$
2500	3.992	$4.9 \cdot 10^{-10}$	$1.53 \cdot 10^{-6}$	3.992	4.157	$2.36 \cdot 10^{-4}$
3000	4.062	$2.61 \cdot 10^{-7}$	$3.23 \cdot 10^{-5}$	4.063	4.223	0.0142
3500	4.127	$2.28 \cdot 10^{-5}$	$2.86 \cdot 10^{-4}$	4.134	4.278	0.268
4000	4.177	$6.95 \cdot 10^{-4}$	$1.44 \cdot 10^{-3}$	4.205	4.327	2.45
4500	4.218	$9.85 \cdot 10^{-3}$	$5.12 \cdot 10^{-3}$	4.304	4.374	13.8
5000	4.253	$8.22 \cdot 10^{-2}$	$1.39 \cdot 10^{-2}$	4.457	4.412	55.4
						0.500
						7.07

It is seen that for oxygen the increase of the energy content, both due to vibrations and to dissociation, begins at much lower temperatures than for nitrogen. At 5000°, the values of  $\beta$  differ by more than 50 per cent. This is due mainly to the smaller dissociation energy and vibrational frequency of  $O_2$ , and to a small extent also to the smaller concentration of  $O_2$  in air (cf. 1.15a).

Table III gives the necessary data for air. We have assumed a composition of

78.05 per cent	Nitrogen
21.00 per cent	Oxygen
0.92 per cent	Rare gases
0.03 per cent	$CO_2$

all percentages being by volume, i.e. by number of molecules. The energy content of the rare gases is  $\beta = 5/2$  because they are monatomic. The  $\beta$  of  $CO_2$  was only guessed because of its small concentration.

From the  $\beta$ 's and  $\alpha$ 's of the constituent gases, the dissociation and the energy content of a mixture are calculated as follows:

$$\alpha = \sum_k c_k \alpha_k \quad (1.17)$$

$$\beta = \frac{\sum_k c_k \beta_k (1 + \alpha_k)}{1 + \alpha} \quad (1.18)$$

where  $c_k$  is the concentration (by volume) of the  $k^{\text{th}}$  component of the mixture ( $\sum_k c_k = 1$ ),  $\alpha_k$  and  $\beta_k$  its degree of dissociation and energy constant, respectively.  $\alpha$  is mainly important for the calculation of  $p/p_0$ , Eq (1.2).

### Specific Heat

The specific heat can be obtained by differentiating the energy content. As long as there is no dissociation, the specific heat per gram at constant pressure is

$$c_p = \frac{d}{dT} (RT\beta) = R(\beta + T \frac{d\beta}{dT}) \quad (1.19)$$

The velocity of sound, again in the absence of dissociation, is given by

$$a^2 = \gamma RT \quad (1.20)$$

where  $\gamma$  is the ratio of the specific heats at constant pressure and constant volume, viz.

$$\gamma = \frac{c_p}{c_v} = \frac{c_p}{c_p - R} \quad (1.21)$$

If  $\beta$  is independent of temperature, we may write from (1.19) and (1.21):

$$\beta = \frac{c_p}{R} = \frac{\gamma}{\gamma - 1} \quad (1.22)$$

as is commonly done in the theory of shock waves and other phenomena involving gases in rapid motion. While this is approximately justified for low temperatures, it is certainly not for air above 600°K.

We have not included the specific heat in our Tables II and III because another numerical differentiation would have been necessary which would have made the results very inaccurate. Moreover, we believed that there was at the moment no pressing need for a table of the specific heat and of the velocity of sound at very high temperatures but that the interest was centered around the shock waves.

If there is dissociation, (1.19) is no longer correct because the energy is  $RT\beta(1 + \alpha)$  and  $\alpha$  as well as  $\beta$  changes with temperature. Moreover, the derivative with respect to  $T$  must now be calculated at constant pressure. Furthermore, the difference between  $c_p$  and  $c_v$  is no longer  $R$  so that (1.21) is no longer valid.

Table III. Energy Content and Dissociation of Air

T N	$c_k \beta_k$ 0	$(1 + \alpha_k)$ Rare gases	$\beta (1 + \alpha)$ $\text{CO}_2$	$\alpha$	$\beta$
300	2.726	0.733	0.023	0.001	3.483
400	2.731	0.739	"	"	3.494
500	2.738	0.745	"	"	3.507
600	2.748 <sub>5</sub>	0.754	"	"	3.527
700	2.764	0.764	"	0.001 <sub>5</sub>	3.552
800	2.781 <sub>5</sub>	0.774	"	"	3.580
900	2.805	0.783 <sub>5</sub>	"	"	3.613
1000	2.829 <sub>5</sub>	0.792 <sub>5</sub>	"	"	3.647
1250	2.889 <sub>5</sub>	0.813	"	0.002	3.727
1500	2.950 <sub>5</sub>	0.829 <sub>5</sub>	"	"	3.805
1750	3.001	0.843	"	"	3.869
2000	3.044	0.855	"	"	3.924
2500	3.115	0.883 <sub>5</sub>	"	0.002 <sub>5</sub>	4.024
3000	3.171	0.949	"	"	4.145
3500	3.227 <sub>5</sub>	1.106	"	"	4.359
4000	3.287	1.400	"	0.003	4.713
4500	3.376 <sub>5</sub>	1.808	"	0.003 <sub>5</sub>	5.211
5000	3.527	2.226	"	0.004	5.780
				0.0000	5.924
				0.0004	4.023
				0.0030	4.133
				0.0121	4.307
				0.0331	4.562
				0.0687	4.875
				0.1058	5.227

Finally, (1.20) ceases to be correct and is replaced by

$$a^2 = \frac{c_p}{c_v} (1 + \alpha + \left[ \frac{\partial \alpha}{\partial \log \rho} \right] T RT) \quad (1.22)$$

## 2. The Approach of Equilibrium between Various Degrees of Freedom of the Molecules.

Suppose the energy content of a mass of gas is suddenly changed, as it is when the gas passes through a shock wave. Then it will take some time until the various degrees of freedom adapt themselves to the new conditions, and this "time" of relaxation" will be different for the different degrees of freedom.

### A. Translation and Rotation.

The equilibrium will be attained most rapidly by the translation. For this degree of freedom, one collision is in general sufficient to come close to equilibrium. In order to have conditions similar to those in a shock wave we may consider a gas of a certain temperature  $T_2$ , into which streams a more dilute gas of a lower temperature  $T_1$ . Then the molecules of the cooler gas will (on the average) become accelerated as soon as they make their first collision with those of the hotter gas. The average kinetic energy of a molecule of a cool gas will increase from  $3/2 kT_1$  in one collision to something of the order  $(3/2 k)^{1/2}(T_1 + T_2)$ .

A shock wave can obviously never be quite discontinuous but the transition from temperature  $T_1$  to  $T_2$  takes place over a distance of at least one gas-kinetic mean free path  $\lambda_t$  ( $t$  for translation). For ordinary gases at room temperature and atmospheric pressure,  $\lambda_t$  is of the order of  $10^{-5}$  cm; it is in first approximation independent of the temperature and inversely proportional to the density; therefore, even a very violent shock wave in which the density increases by a factor 6 to 10 (cf. par. 3 Table VIII), must have an extension of at least about  $10^{-6}$  cm. The classical theory of the physical structure of shock waves as given by Becker (Zeits. f. Phys. 8, 321, 1922) gives extremely small extensions which become of the order of  $10^{-7}$  cm for very violent waves. The theory of Becker which takes into account the heat conduction but neglects molecular effects can therefore

not be correct, at least not for violent shock waves. Becker, himself, pointed out that the problem requires a treatment based on the kinetic theory of gases. In practice a spatial extension of the shock wave of the order of one mean free path is, of course, of no importance at all, even at rather low initial pressures.

The molecular rotation may approach equilibrium as rapidly as the translation. This would be expected for strongly elongated molecules such as CO<sub>2</sub>. If the effective boundary of the molecule is nearly spherical (e.g. N<sub>2</sub> or S<sub>2</sub>) the excitation of molecular rotations may be estimated to take roughly 10 to 100 collisions. To show that the rotation approaches equilibrium so quickly, we use the results of Landau and Teller, Physik. Zeits. d. Sowjetunion 10, 34(1936). These authors have found that the effectiveness of collisions on a certain degree of freedom is determined by the ratio

$$\chi = \tau_c / \tau_0 \quad (2.1)$$

where  $\tau_c$  is the effective duration of the collision and  $\tau_0$  the natural period of the degree of freedom concerned. If  $\chi$  is of order unity or smaller, one or a few collisions will be sufficient to establish equilibrium whereas a large number of collisions is required if  $\chi \gg 1$  (cf. 2.5).

$\tau_c$  in (2.1) may generally be written

$$\tau_c = s/v \quad (2.2)$$

where  $v$  is the relative velocity of the two colliding molecules and  $s$  the range of the intermolecular forces, i.e. the distance over which the molecules interact strongly. We may expect  $s$  to be of the order of one half to one Bohr radius, i.e. 2.5 to  $5 \cdot 10^{-9}$  cm, a range of values which seems confirmed by some experimental results on the approach of vibrational equilibrium (cf. Table IV). In the case of rotation  $\tau_0$  may be taken as the time required for one revolution, or rather this time divided by  $2\pi$  (cf. 2.4) so that  $\tau_0 = r/v_r$  where  $r$  is the radius of the molecule (distance of an atom from the center of gravity) and  $v_r$  is the velocity of

the atoms in their revolution around the center of gravity. Now  $v_r$  is of the same order as  $v$ , the velocity of molecular translation (equipartition of energy!) and  $r$  is of the same order as  $s$ . Therefore  $\chi$  is of order unity for rotation, and equilibrium between rotations and translation will be attained in a few collisions.

We shall find in the following that all other degrees of freedom behave quite differently in that many collisions are necessary to establish equilibrium. Therefore it will be convenient to group together translation and rotation on one side, and all other degrees of freedom on the other. The latter we shall call the "inert" degrees of freedom while translation and rotation will be denoted as the "active" degrees of freedom. For all practical purposes we may say that the energy content of the active degrees of freedom can change almost discontinuously, because a distance of a few mean free paths may be considered negligible. We can then define the temperature of a moving gas at each point by the energy content of the active degrees of freedom, which is

$$E_a + p/\rho = \beta_a p/\rho = \beta_a RT \quad (2.3)$$

(the last relation being only valid if there is no dissociation). In (2.3)  $\beta_a$  is independent of the temperature and equal to  $5/2$  for monatomic,  $7/2$  for diatomic gases (cf. par. 1). The energy content of the inert degrees of freedom,  $E_i$ , on the other hand, cannot change abruptly and is therefore not always in equilibrium with that of the active ones; in other words,  $E_i$  is not necessarily related to the local temperature  $T$  in the way discussed in par. 1.

### B. Vibrations

#### Theory

The most important inert degree of freedom are the vibrations. For these, we set in (2.1)

$$\tau_o = 1/2 \pi \nu \quad (2.4)$$

where  $\nu$  is the natural frequency of the molecular vibration. (In all formulae like (2.1)  $2\pi\nu$  rather than  $\nu$  should be used as representing the frequency because the frequency is generally introduced into physical formulae by taking the time derivative of expressions like  $\sin 2\pi\nu t$ . If we took  $\nu$  instead of  $2\pi\nu$  in (2.4), the only change would be that the values of  $s$  deduced from experimental data would be multiplied by  $2\pi$ ). Since the frequencies of molecular vibrations are rather high, it is plausible that  $\chi$  is rather large; this will be shown by direct calculation and by discussion of experimental results below. For the case  $\chi \gg 1$ , Landau and Teller give the formula

$$p_{10} = Ce^{-\chi} \quad (2.5)$$

Here  $p_{10}$  is the probability that a molecule in the first excited state of vibration is de-excited by a collision with another molecule.  $C$  is a geometrical factor which gives the probability that the collision of the two molecules will take place in a direction suitable for excitation or de-excitation of the vibration. There are no experimental data sufficiently accurate to deduce  $C$ , so that qualitative arguments must be used for its determination. Obviously,  $C$  must be less than unity, and probably it will lie between  $1/3$  and  $1/30$  in most cases, its value being higher for diatomic and lower for polyatomic molecules because it is less likely that a complicated molecule is hit at the right place to induce a given mode of vibration. In our computations below, we shall use arbitrarily  $C=1/10$ .

Presumably, a better approximation could be obtained by introducing in (2.5) another factor, viz. a certain power of  $\chi$ . Arguments can be given for a factor  $\chi^{-2}$ . However, these arguments are too uncertain to justify at present the inclusion of such fine points.

The most important factor in (2.3) is the exponential  $e^{-\chi}$  where (cf. 2.1, 2.2, 2.4)

$$\chi = 2\pi\nu s/v \quad (2.6)$$

Let us investigate  $\chi$  for the case when the kinetic energy of the relative motion of the colliding molecules is just  $kT$ , i.e.

$$\frac{1}{2} M v^2 = kT \quad (2.7)$$

where  $M$  is the reduced mass of the two molecules; if they are equal,  $M$  is one half the mass of one molecule. The value of  $\chi$  for the velocity determined by (2.7) is

$$\chi_1 = 2\pi \nu s \sqrt{M/2kT} \quad (2.8)$$

This can be re-written as follows:

$$\chi_1 = \sqrt{h/2kT} \cdot s \sqrt{\frac{4\pi^2 M \nu}{h}} \quad (2.9)$$

For the collision of two equal diatomic molecules, each consisting of two equal atoms,  $M$  is the mass of one atom; then the reciprocal of the last factor is (2.9) viz

$$b = \sqrt{h/4\pi^2 M \nu} \quad (2.10)$$

represents the amplitude of the molecular vibration in the lowest quantum state. Generally, the  $b$  defined in (2.10) has the value

$$b = \frac{8.2 \cdot 10^{-8}}{\sqrt{\mu \nu}} \text{ cm} \quad (2.10a)$$

where  $\mu$  is the molecular weight of the molecule (assuming collision between equal molecules) and  $\nu$  the vibrational frequency in  $\text{cm}^{-1}$ . For  $\text{N}_2$ ,  $\nu = 2345$  and  $\mu = 28$  so that  $b = 3.1 \cdot 10^{-10} \text{ cm}$ . Thus we see that  $b$  is very small compared with the range  $s$  of the forces. The factor  $\sqrt{h\nu/2kT}$  in (2.9) is also in general greater than unity, so that  $\chi_1$  is indeed very large compared with unity as we expected above. Therefore (cf. 2.5) the probability of transfer of energy between vibration and

translation is very small; the vibration is an inert degree of freedom. It is seen from the derivation that the reason for this result is not so much that the energy of one vibrational quantum  $h\nu$  is large compared with the average energy of translation,  $kT$ , but rather that the amplitude of the vibrations,  $b$ , is very small compared with the range  $s$  of the intermolecular forces. This in turn is due to the large elastic forces which govern the elastic vibrations.

The quantity  $\chi$  (2.6) will be reduced, and therefore the probability of energy transfer  $P_{10}$  (2.5) considerably increased, if we take higher velocities  $v$ . Therefore a given molecule will lose and gain vibrational energy mostly at the times when its kinetic energy of translation is high compared with  $kT$ , i.e. when it is in the tail of the Maxwell distribution. If we average over all the molecules in the gas, the probability of energy transfer per collision becomes

$$P_{10} = 2/\sqrt{\pi} \int e^{-x} \sqrt{x} dx C e^{-\chi} \quad (2.12)$$

where

$$x = \frac{M v^2}{2kT} \quad (2.12a)$$

(2.12) represents the probability (2.5), averaged over the Maxwell distribution of the relative velocities of the two colliding molecules.\* With (2.6) for  $\chi$ , the integration of (2.12) can be carried out by the saddle point methods, the integrand having a steep maximum near

\* It might be preferable to take into account the different collision probability of fast and slow molecules, i.e. to replace (2.12) by

$$P_{10} = \int e^{-x} x dx C e^{-\chi} \quad (a)$$

which would give instead of (2.13)

$$P_{10} = 2/9 \sqrt{\pi} \sigma^{3/2} e^{-\sigma} \quad (b)$$

The temperature dependence of  $P_{10}$  would not be changed very much by this correction because the difference between (b) and (2.13) would be largely compensated by a different value of  $s$  deduced from the experiments.

$$x_0 = 1/2 (2\pi s \nu)^{2/3} (M/kT)^{1/3} \quad (2.12b)$$

The integration gives

$$P_{10} = C' \sigma e^{-\sigma} \quad (2.13)$$

where  $\sigma = 3x_0 = 3/2 (s/b)^{2/3} (h\nu/kT)^{1/3}$  (2.14)

$$C' = \frac{4}{(3)}^{1/2} C \quad (2.14a)$$

( $b$  as defined in (2.10, 2.10a),  $s$  the range of the molecular forces,  $\nu$  the frequency of vibration). (Eqs. (2.13, 14) are similar to the equations determining the rate of nuclear reactions in stars).

Numerically, (2.14) may be written

$$\sigma = 0.090 (\nu s)^{2/3} (\mu/T)^{1/3} \quad (2.15)$$

where  $\nu$  is measured in  $\text{cm}^{-1}$ ,  $s$  in units of  $10^{-9} \text{ cm}$ ,  $T$  in degrees Kelvin, and  $\mu$  is the molecular weight per molecule (or twice the reduced molecular weight,  $2\mu_A\mu_B/(\mu_A + \mu_B)$ , if two unequal molecules collide).

We shall now try to get a more quantitative estimate of  $s$ . Experiments are available (cf. below), among other gases, for pure  $\text{CO}_2$ , and for the action of  $\text{N}_2$  on the vibrations of  $\text{O}_2$ . For  $\text{CO}_2$ , Fricke (Journ. of the Acoust. Soc. of Am. 12, 245(1940)) finds that  $Z = 86,000$  collisions are necessary for de-excitation of the first excited vibrational state, so that

$$P_{10} = \frac{1}{Z} = \frac{1}{86,000} = 1.15 \cdot 10^{-5}$$

Taking  $C' = 1/10$ , (2.13) gives  $\sigma = 11.5$ . Using this number in (2.15) with  $\nu = 667 \text{ cm}^{-1}$ , we find,

$$s = 5.6 \cdot 10^{-9} \text{ cm. } (\text{CO}_2) \quad (2.16a)$$

For the de-excitation of the vibrations of  $O_2$  by collisions with  $N_2$ , Kneser and Knudsen find  $P_{10} = 10^{-5}$ . Inserting this figure in (2.13, 15) and taking  $\nu = 1570 \text{ cm}^{-1}$ , we obtain

$$S = 3 \cdot 10^{-9} \text{ cm } (O_2/N_2) . \quad (2.16b)$$

Both the results (2.16a) and (2.16b) are of the order of the Bohr radius as we assumed above. Differences between the values of  $s$  for different molecules are, of course, to be expected. We can therefore not predict the value of  $s$  for a pair of molecules for which it has not been measured experimentally. This is very unfortunate because  $P_{10}$ , or

$$Z = 1/P_{10} , \quad (2.17)$$

is very sensitive to  $s$ . This can be seen directly from (2.13, 14) or from Table IV in which we have calculated  $Z$  from (2.13, 14) for  $O_2$  and  $N_2$ , in each case for two different values of  $s$ . A more detailed discussion of Table IV will be given in par. 2D.

#### Influence of foreign gases, experimental difficulties.

Collisions between two different molecules are often more effective in transferring energy to and from the vibrations than collisions between like molecules. This is the case especially (1) if the two colliding molecules have a chemical affinity and (2) if one molecule is very light so that its velocity is great. In case (2) which is realized for  $H_2$ , He, etc.,  $\mu$  in (2.15) is very small. In case (1) the interaction between the two molecules is much more intense than usually which may perhaps result in more sudden changes of interaction and correspondingly shorter effective range, or even in a complete failure of the Landau-Teller theory when the two molecules penetrate so deeply into each other that they can be said to form a temporary compound. In the latter case, the temperature dependence may be quite different from that indicated in (2.13).

Table IV. Theoretical Temperature Dependence of the Number of Collision Necessary for  
De-excitation of the First Vibrational State.

Temperature °K)			300	500	700	1000	1500	2000	3000	5000
<b>Vibrating Molecule</b>										
CO <sub>2</sub>	5.6·10 <sup>-9</sup>	$\sigma$	11.20	9.45	8.45	7.50	6.55	5.95	5.20	4.38
		Z	65,000	13,500	3500	2400	1080	650	340	180
O <sub>2</sub>	4·10 <sup>-9</sup>		14.32	12.08	10.80	9.58	8.37	7.60	6.56	5.30
		Z	1.1·10 <sup>6</sup>	1.4·10 <sup>5</sup>	46,000	15,000	5100	2600	1150	380
	3·10 <sup>-9</sup>	$\sigma$	11.82	9.97	8.91	7.91	6.91	6.28	5.49	4.62
		Z	1.1·10 <sup>5</sup>	21,500	8400	3400	1450	850	440	220
N <sub>2</sub>	3·10 <sup>-9</sup>	$\sigma$	14.78	12.48	11.14	9.89	8.64	7.85	6.75	5.77
		Z	1.7·10 <sup>6</sup>	2.0·10 <sup>5</sup>	62,000	20,000	6600	3200	1400	570
	2.5·10 <sup>-9</sup>	$\sigma$	13.08	11.05	9.88	8.77	7.66	6.96	6.08	5.11
		Z	3.7·10 <sup>5</sup>	57,000	19,500	7500	2700	1500	720	320
<u>Collisions with H<sub>2</sub>O</u>										
O <sub>2</sub>	0.93·10 <sup>-9</sup>	Z	400	210	140	100	75	60	50	40
N <sub>2</sub>	"	Z	1300	650	320	200	130	100	75	50

As will be seen from Table V, the foreign gases investigated are 3 to 4000 times more effective in de-exciting the vibration of  $O_2$  than  $O_2$  itself, the effect being greatest for complicated molecules such as  $C_2H_2OH$  which has a chemical affinity to  $O_2$ , and for water, which can probably form a temporary compound with  $O_2$ . The effect of  $N_2$  on  $O_2$  is almost as small as that of  $O_2$  itself because there is not much chemical interaction; the collisions between  $O_2$  and  $N_2$  will be discussed in more detail in par. 2D.

The large effect of water vapor on the variation of oxygen makes it extremely difficult to measure the small effect of collisions between  $O_2$  molecules themselves. Only a lower limit for  $Z$  was therefore obtained in the experiments on "pure"  $O_2$ , viz. 500,000.

For the problem of shock waves we must conclude that the establishing of vibrational equilibrium will depend sensitively on the humidity of the air. On hot humid days, the water vapor content of the air may easily reach 3 per cent (23 mm vapor pressure) so that only  $400/0.03 = 13,000$  collisions would be necessary to establish vibrational equilibrium for the oxygen. On the other hand, for completely dry air the necessary number of collisions is about  $10^5$  because then only the collisions with nitrogen will be important. A more accurate discussion of the humidity effect will be given in Table VI.

Excitation and De-excitation. Instead of the probability  $P_{10}$  of de-excitation per collision, it is convenient to introduce the probability  $k_{10}$  of de-excitation per second which is given by

$$k_{10} = P_{10} \cdot N = N/Z \quad (2.18)$$

where

$$N = N_g v \quad (2.18a)$$

is the number of collisions per second,  $N$  the number of molecules per  $cm^3$ ,  $g$  the gas-kinetic collision cross section and  $v$  the average relative velocity of two

colliding molecules, viz.  $\sqrt{\frac{8}{\pi} \frac{kT}{M}}$ . The quantity  $k_{10}$  has two advantages compared with  $P_{10}$ , viz. (1) that it is more directly related to the extension of the shock wave and (2) that it is directly connected with observational data (cf. 2.22, 26) whereas the connection of  $P$  with these data involves the somewhat uncertain cross section  $q$ .

The probability of excitation,  $k_{01}$ , is connected with the probability of de-excitation,  $k_{10}$ , by the statistical principle of detailed balancing according to which

$$k_{01} = k_{10} e^{-\frac{h\nu}{kT}} \quad (2.19)$$

The time rate of change of the number  $y_0$  of molecules without vibration is then

$$\frac{dy_0}{dt} = k_{10} y_1 - k_{01} y_0 \quad (2.19a)$$

where  $y_1$  is the number of molecules in the first excited vibrational state. Similar equations hold for the other  $y_n$  where, according to quantum theory,  $k_n, n=1 = nk_{10}$  and  $k_{n-1}, n = k_{n,n-1} e^{-h\nu/kT}$ . By adding the equations for the various  $y_n$ , an equation for the total energy of vibration,

$$E_v = h\nu \sum_{n=0}^{\infty} n v_n \quad (2.19b)$$

can be obtained, namely

$$\frac{dE_v}{dt} = k_{10} (1 - e^{-h\nu/kT}) (E'_v - E_v) \quad (2.20)$$

Here  $E'_v$  is the vibrational energy in thermal equilibrium, viz.

$$E'_v = \frac{h\nu}{e^{h\nu/kT}-1} \quad (2.20a)$$

Eq. (2.20) is valid no matter how large the deviation from thermal equilibrium. The factor  $1 - e^{-hv/kT}$  takes account of the fact that there occur transitions away from equilibrium as well as towards equilibrium. The solution of (2.20) is

$$E'_v - E_v = Ae^{-\omega_0 t} \quad (2.21)$$

where  $\omega_0$  is the reciprocal of the time of relaxation and is given by (cf. 2.20).

$$\omega_0 = k_{10} (1 - e^{-hv/kT}) \quad (2.22)$$

It has been assumed in (2.21) that T remains constant. This is not strictly correct in shock waves (cf. par. 3,4) where  $\omega_0$ , being a function of T, will change with time so that the integral of (2.20) cannot be given in closed form.

In shock waves, we are interested in the spatial variation of  $E_v$ . If the gas flows with a velocity v, we may write

$$\frac{dE_v}{dx} = \frac{1}{v} \frac{dE_v}{dt} = \frac{E'_v - E_v}{\lambda_v} \quad (2.23)$$

where

$$\lambda_v = v \omega_0 \quad (2.24)$$

defines the mean free path for vibration.

Evaluation of Experiments. The experimental determination of  $\omega_0$  is based upon the absorption and dispersion of sound in gases. The theory of this phenomenon has been given by H. O. Kneser, Ann. d. Phys. 16, 337 (1933) and Journ. Acoust. Soc. Amer. 5, 122 (1933), and others. The absorption coefficient  $\mu$  per wave length depends on the circular frequency  $\omega$  of the sound wave approximately\* as

\* In order to obtain (2.25),  $c_p - c_{pa}$  must be assumed to be small in comparison with  $c_p$ . Since  $\mu$  is the absorption coefficient per wave length, the absorption coefficient per centimeter will behave as  $\frac{\omega^2}{\omega_{max}^2 + \omega^2}$  and will therefore obtain its maximum value for  $\omega = \infty$ .

$$\mu \approx \frac{\omega}{\omega_{\max}^2 + \omega^2} \quad (2.25)$$

where  $\omega_{\max}$  is the frequency of maximum absorption per wave length.  $\omega_{\max}$  can be determined experimentally, and  $\omega_0$  may be deduced from it using the relation

$$\frac{\omega_0}{\omega_{\max}} = \frac{c_{pa} (c_{pa} - R)}{c_p (c_p - R)} . \quad (2.26)$$

Here  $c_p$  is the ordinary specific heat at constant pressure and  $c_{pa}$  the specific heat counting the "active" degrees of freedom only. In contrast to (2.25), (2.26) is exact.

Experimental Results. Experiments were made by H. O. Kneser and V. O. Knudsen, Ann. d. Physik 21, 682 (1935) on the vibrations of  $O_2$ , by Fricke and by Knudsen and Fricke, Journ. Acoust. Soc. Amer. 12, 245 and 255 (1940) on  $CO_2$  and a few other gases, and by Küchler, Zeits. f. phys. Chemie B 41, 199 (1938), on the temperature dependence of the time of relaxation. The latter experiments were probably carried out with somewhat impure gases because Küchler finds for  $CO_2$  at room temperature  $Z = 50,000$  whereas Fricke gives 86,000 (impurities reduce  $Z$ , cf. above and Table V), and a similar discrepancy exists for  $N_2O$  (7,500 vs. 11,800). The experiments of Kneser and Knudsen were the first systematic ones carried out and were therefore less accurate than the later work of Knudsen and Fricke, but the results of Kneser and Knudsen are most important for us because they were done with oxygen. For  $N_2$  there are no experiments but only an estimate by P. S. H. Henry, Nature 129, 200 (1932) based on the failure to detect the influence of the vibrational specific heat on the velocity of sound in certain experiments. Henry estimates  $\omega_0 \approx 10^4$  sec<sup>-1</sup>, i.e.  $Z \approx 10^6$  for  $N_2$  which seems not implausible.

Table V gives some of the experimental results. They bear out the features discussed above and expected theoretically, viz.

Table V Experimental Results on the Excitation of Molecular Vibrations. Number of Collisions Required for De-excitation, Z, and Reciprocal Time of Relaxation,  $\omega_0$  (in sec<sup>-1</sup>), for Various Molecules Colliding with other Molecules.

Collision with	O <sub>2</sub>	N <sub>2</sub>	H <sub>2</sub>	CO <sub>2</sub>	H <sub>2</sub> O	H <sub>2</sub> S	CH <sub>3</sub> OH	C <sub>2</sub> H <sub>5</sub> OH
Vibration of O <sub>2</sub> (Knudsen and Kneser)	Z $\omega_0$	> 500,000 $< 3 \cdot 10^3$	100,000 $5 \cdot 10^4$	20,000 $5 \cdot 10^5$	25,000 $1.7 \cdot 10^5$	400 $1.1 \cdot 10^7$	4,200 $1.3 \cdot 10^6$	---
								120 $6 \cdot 10^7$

Vibration of CO <sub>2</sub> (Kneser and Fricke)	Z $\omega_0$	----	-----	215 $8.0 \cdot 10^7$	86,000 $9.8 \cdot 10^4$	17 $1.02 \cdot 10^9$	1,200 $1.14 \cdot 10^7$	36 $3.1 \cdot 10^8$	-----
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The same quantities for some pure gases (Fricke)

Gas	O <sub>2</sub>	CO <sub>2</sub>	N <sub>2</sub> O	COS	CS <sub>2</sub>	SO <sub>2</sub>
Z	> 500,000	86,000	11,800	9,600	8,700	1,900
$\omega_0$ (in $10^5$ sec <sup>-1</sup> )	< 0.08	0.98	6.9	11.5	14.3	55

Z for CO<sub>2</sub> at various temperatures (Küchler)

T(degrees Kelvin)	293	373	473	573	673
Z	50,000	31,000	19,000	12,000	9,000

Ratio of Z<sub>293°</sub>/Z<sub>673°</sub> for various gases (Küchler)

Colliding gases	CO <sub>2</sub> - CO <sub>2</sub>	N <sub>2</sub> O - N <sub>2</sub> O	CO <sub>2</sub> - H <sub>2</sub>	CO <sub>2</sub> - H <sub>2</sub> O
Z <sub>293°</sub>	50,000	7,500	300	105
Z <sub>293°</sub> /Z <sub>673°</sub>	5.6	3.6	1.0	0.4

1. All the pure gases investigated have rather high Z (small  $\omega_0$ , long relaxation times), the smallest being  $\text{SO}_2$  with  $Z \approx 2,000$ , the largest  $\text{O}_2$  with  $Z > 500,000$ . The large value for  $\text{O}_2$  is probably due mostly to its high vibration frequency. The decrease of Z from  $\text{CO}_2$  to  $\text{COS}$  to  $\text{CS}_2$  is also in the direction of decreasing  $\omega$ ; on the other hand, the small value for  $\text{SO}_2$  is presumably due to the greater chemical activity of that molecule.

2. The impurities investigated gave smaller Z than pure gases. It cannot be decided at present whether this is due to the selection of gases used in the experiments, or to a general rule. Among diatomic molecules,  $\text{H}_2$  is most effective in de-exciting  $\text{O}_2$  and  $\text{CO}_2$ ; this is to be expected theoretically from its small mass (large velocity). Triatomic gases are on the whole more effective than diatomic ones; this may be due to the fact that there will always be some "corner" of a triatomic molecule which has a chemical affinity or at least a strong interaction with a given molecule. Among the triatomic gases, there is again a decrease of Z with increasing chemical activity ( $\text{CO}_2$  to  $\text{H}_2\text{S}$  and  $\text{H}_2\text{O}$ ). Polyatomic molecules are even more effective than triatomic ones, for the same reason.

By collisions with the same molecule, the vibrations of  $\text{CO}_2$  are in general more affected than those of  $\text{O}_2$ , because of the smaller frequency of vibration.

3. The temperature dependence of Z for  $\text{CO}_2$  is about as expected (cf. Table IV). Generally, the decrease of Z with increasing temperature is most pronounced if Z is large, in agreement with theoretical expectation. Whether the increase of Z with the temperature as found by Kuchler for collisions between  $\text{CO}_2$  and  $\text{H}_2\text{O}$ , is real cannot be decided at present; however, Z is very small in this instance so that the Landau-Teller theory can probably not be applied.

Several Degrees of Freedom. At first sight, it might be expected that each mode of vibration has its own relaxation time, this time being greater for the modes with higher frequency. Experiments show, however, that this is not the

case because all the experimental curves show only one absorption maximum with the absorption coefficient falling off on both sides according to (2.25). This behavior can easily be understood if we remember that the resolution of the vibration into normal modes is only an approximation which is correct only for exactly harmonic forces. The anharmonicity will mix the various normal modes in each vibrational quantum state. An extreme case of mixing is known in CO<sub>2</sub> where the second excited state (vibrational quantum number\*  $n_1 = 2$ ) of the first mode of vibration ( $\nu_1 = 667 \text{ cm}^{-1}$ ) is degenerate with the first quantum state of the second mode ( $\nu_2 = 1336 \text{ cm}^{-1}$ ) ( $n_2 = 1$ ) (cf., e.g., Sponer, loc. cit.). The anharmonicity causes an "interaction" of the two resonating quantum states with the result that a splitting occurs into two states of considerably different frequency (1286 and 1388 cm<sup>-1</sup>). The form of vibration in each of these states is a combination of modes 1 and 2 with about equal amplitudes.

In other molecules, the mixing of different modes is usually less strong but it must always exist to some extent. Let us assume, e.g., that there is a mode of vibration with a high frequency  $\nu_2$  which is between 3 and 4 times the frequency  $\nu_1$  of another mode. Then the first excited state of mode 2 ( $n_2 = 1$ ) will contain some admixture of the fourth state of mode 1 ( $n_1 = 4$ ). In this case, the excitation of the state  $n_2 = 1$  will not take place by direct transfer of energy from the translation, but the translation will excite in successive collisions the states  $n_1 = 1, 2$  and 3, and finally, in a fourth collision, the state  $n_2 = 1$ . This mechanism avoids large energy transfers in one collision which are very improbable according to the Landau-Teller theory (cf. 2.15). The transition from  $n_1 = 3$  to  $n_2 = 1$  is somewhat less probable than a collision in which  $n_1$  is raised by one unit because the mixing between  $n_2 = 1$  and  $n_1 = 4$  is assumed small; on the other hand, it is more probable because the energy difference between  $n_2 = 1$

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\* In order to avoid confusion with the velocity  $v$ , we denote the vibrational quantum number by  $n$  rather than the customary  $v$ .

and  $n_1 = 3$  is smaller than  $\nu_1$ . The Z for the transition  $n_1 = 3$  to  $n_2 = 1$  is therefore probably of the same order or smaller than for the excitation of the first mode, and it can therefore be understood that only the successive excitation of quantum states of the lowest mode of vibration gives rise to an observable absorption of sound.

### C. Dissociation

The dissociation differs from other degrees of freedom in that it becomes appreciable at temperatures at which  $kT$  is still very small compared with the dissociation energy D per molecule. We have mentioned in part I that  $\frac{D}{kT} = \frac{59,000}{T}$  for oxygen and  $91,600/T$  for nitrogen. On the other hand, we have shown in Table II that the degree of dissociation is as much as 1.4 per cent for  $O_2$  at  $3000^\circ K$  and for  $N_2$  at  $5000^\circ K$ . At these temperatures,  $D/kT$  is about 20 in both cases, and the Boltzmann factor  $e^{-\frac{D}{kT}} \approx e^{-20} \approx 10^{-9}$ . The fact that an appreciable dissociation is possible for such a small Boltzmann factor is due to the large a priori probability of the dissociated states.

In order to produce dissociation, two molecules must collide which have a relative kinetic energy at least equal to D. Such molecules are very rare because of the small Boltzmann factor  $e^{-\frac{D}{kT}}$ . Dissociation will therefore take a considerable time at  $3000-5000^\circ K$  even if every collision between molecules of sufficient energy is effective.

The same conclusion can be reached by considering the inverse process, viz. recombination. In order that two atoms recombine into a molecule, there must be a triple collision between the two atoms and another molecule which takes up the excess energy and momentum. Triple collisions, however, are rare events especially if two of the colliding particles must be atoms which are relatively rare as long as the degree of dissociation remains low.

We must now examine the efficiency of collisions between two molecules of sufficient relative velocity in causing dissociation of one of the molecules.

If two molecules have relative kinetic energy equal to  $D$ , i.e. several electron volts, they will penetrate very deeply into each other. In this case, we can no longer distinguish between fast motions (of the electrons) and slow motions (of the molecules as a whole), and we can therefore no longer conclude that the transfer of energy from the slow molecular translation to the fast electronic motion is improbable. It is very difficult to make any quantitative estimates but we believe that the efficiency of collisions between molecules of energy greater than  $D$  will not be reduced by a factor of the type of (2.5) but will be determined mainly by a geometrical factor which may perhaps be somewhat smaller than for the excitation of vibrations. In numerical calculations, we shall assume an efficiency  $C_d = 1/100$  which may be wrong by a factor of 10 or more either way.

The probability that the relative kinetic energy of a pair of molecules is between  $kT_x$  and  $kT(x + dx)$ , is given by the Maxwell distribution

$$\sqrt{\frac{2}{\pi}} \sqrt{x} dx e^{-x}$$

The velocity of the molecules in question is  $\frac{\sqrt{\pi}}{2} \sqrt{x}$  times the average relative velocity  $\bar{v}$  of two molecules. Therefore, the fraction of all molecular collisions for which the relative kinetic energy of the colliding molecules lies in the interval mentioned, is approximately

$$f(x)dx = e^{-x} x dx \quad (2.27)$$

The fraction of collisions for which

$$x > x_0 \equiv \frac{D}{kT} \quad (2.27a)$$

is then

$$F(x_0) = \int_{x_0}^{\infty} f(x)dx = e^{-x_0} (x_0 + 1) \approx x_0 e^{-x_0} = \frac{D}{kT} e^{-D/kT} \quad (2.27b)$$

Therefore, the number of ordinary molecular collisions required per dissociation, is

$$Z_d = \frac{1}{C_d F(x_0)} = \frac{1}{C_d} \frac{e^{x_0}}{x_0} \quad (2.28)$$

where  $C_d$  is the efficiency of the collisions between molecules of sufficient energy in producing dissociation. The reciprocal relaxation time for dissociation is

$$\omega_d \approx \frac{N}{Z_d d} \quad (2.29)$$

where  $N$  is the number of collisions per second (cf. 2.18, 2.18a). The mean free path for dissociation is (cf. 2.24).

$$\lambda_d = y/\omega_d \quad (2.29a)$$

Because of the large factor  $e^{x_0}$ , the number of collisions required for dissociation is very large at temperatures of 3000-5000° K. at which the dissociation of air becomes important (Tables II and III). In Table VII (cf. p. 52a) we give the values of  $Z_d$ ,  $\omega_d$ , and  $\lambda_d$  for oxygen and nitrogen; it is seen that  $Z_d$  lies between  $10^6$  and  $10^{12}$  and is thus much higher than for the vibration. It is obvious that impurities cannot greatly affect  $Z_d$  because the decisive factor is the Boltzmann factor rather than the efficiency of the collisions.

#### D. Conclusions on the Excitation of Air.

##### Vibrations

Neither the theory nor the available experimental results are sufficiently accurate to permit any quantitative predictions on the mean free path for the vibrations of the most important gases,  $O_2$  and  $N_2$ . It is certain that these mean free paths are rather long, and under certain circumstances they may become comparable with the dimensions of a projectile.

Experimental information is available (Table V) only on the effect of  $N_2$  and of water vapor on the vibration of  $O_2$ ; in addition an upper limit is known for the effect of  $O_2$  on the  $O_2$  vibration. The effect of  $N_2$  on  $O_2$  is described by an effective range  $s = 3 \cdot 10^{-9} \text{ cm}$  as computed in (2.18a). In Table IV, we have calculated  $Z$  as a function of temperature with this value of  $s$ . These calculated values should represent the temperature dependence of the effect of  $N_2$  on the vibrations of  $O_2$  fairly accurately, i.e., within a factor of perhaps 3.

For the collisions between two  $O_2$  molecules, the experiments give  $Z > 500,000$  at room temperature. Assuming  $Z = 10^6$ , we obtain  $s = 4 \cdot 10^{-9} \text{ cm}$  from (2.13, 15). The values of  $Z$  for  $O_2$  at various temperatures with  $s = 4 \cdot 10^{-9}$  are also given in Table IV; the actual  $Z$  for  $O_2 - O_2$  collisions may be smaller than the values given in the table by about a factor of 2, but greater by any amount. In any case, in air the vibrations of  $O_2$  will be excited much more easily by collisions with  $N_2$  than by collisions with other  $O_2$  molecules, both because of the greater abundance of  $N_2$  and of the smaller  $Z$ .

In Table VI we give the estimated times and distances required to establish equilibrium of the molecular vibrations in air. In particular, Table VI A gives the reciprocal time of relaxation,  $\omega_0$ , as a function of temperature for various assumptions.  $\omega_0$  has been calculated from (2.18, 18a and 22), considering  $q$  as independent of the temperature. The values of  $q$  were obtained by comparing the values of  $Z$  and  $\omega_0$  given by Kneser and Kunze for room temperature; these  $q$ 's seem somewhat low but the errors are not important compared with the uncertainties in the theory. The density of the air was assumed to be  $1.18 \cdot 10^{-3}$ , corresponding to atmospheric pressure at 300°K. In the first row of Table VI A,  $\omega_0$  is given for the vibrations of  $O_2$ , taking into account only the collisions with  $N_2$  molecules. The neglected collisions with  $O_2$  can increase  $\omega_0$  by 10 per cent at most.

Collisions with water molecules are very effective in exciting the vibrations of  $O_2$  (Table V). Four hundred collisions with  $H_2O$  are sufficient for de-excitation of  $O_2$  at room temperature; therefore, as little as one per cent of water

vapor will be three times as effective as all the nitrogen in the air. In the second row of Table VI A we have listed the value of  $\omega_0$  for collisions of  $O_2$  molecules with  $H_2O$ , assuming a concentration of 1 per cent water vapor by volume. On hot humid days, the water concentration may be easily 3 per cent. It is seen that, at 1 per cent, the collisions with  $H_2O$  are more effective than those with  $N_2$  at 500° K, but less effective at 700° and higher temperatures. This behavior is due to the fact that  $\omega_0$  rises very rapidly with temperature for collisions with  $N_2$ , but rather slowly for collisions with  $H_2O$ . (Table IV)

While the information obtainable on  $O_2$  is fairly satisfactory, very little can be said about the excitation of the vibrations of  $N_2$ . It is reasonable to expect that the effect of  $O_2$  on the  $N_2$  vibrations can be described by the same effective range,  $s = 3 \cdot 10^{-9}$  cm, as the effect of  $N_2$  on  $O_2$ , although this is by no means certain. In Table IV we have given the corresponding  $Z$  for  $N_2$ ; it is much higher than the  $Z$  for  $O_2$  with the same  $S$  because the vibration frequency of  $N_2$  is about 50 per cent higher than for  $O_2$ . The third row of Table VI gives  $\omega_0$  for the excitation of the vibration of  $N_2$  in air, assuming that only collisions with  $O_2$  are effective. These values for  $\omega_0$  can therefore be regarded as lower limits.

No experimental results are available concerning the effect of collision with the  $N_2$  molecules on the vibration of  $N_2$ . To obtain any theoretical estimate, we must find an interpretation of the difference between the effective range  $s$  for  $O_2 - O_2$  and  $O_2 - N_2$  collisions, viz.  $s \approx 4 \cdot 10^{-9}$  and  $s = 3 \cdot 10^{-9}$  cm, respectively. There are two possible interpretations: The first alternative is to assume that generally collisions between different molecules are more effective than between equal ones. Such a tendency seems to exist in the experimental result (Table V) but there appears to be no theoretical justification. Moreover, it is to be remembered that the experiments were mostly done with polyatomic molecules, for

which there are other reasons for a stronger interaction (cf. point 2 in the section on Experimental Results of par. 28). Thus we do not get an explanation for the effectiveness of the collisions between  $O_2$  and  $N_2$ , and we are led to the second alternative. This is based on the fact that  $N_2$  is a more compact molecule than  $O_2$ , having a greater binding energy and smaller distance between the atoms. From this difference in structure we may expect a shorter range of the forces for  $N_2$  which would explain the smaller value of  $s$  for  $O_2 - N_2$  collisions as compared with  $O_2 - O_2$ .

If this second alternative is accepted, we should expect an even smaller  $s$  for the interaction between two  $N_2$  molecules than for the  $N_2 - O_2$  interaction. We have therefore included in Table IV the values of  $Z$  for  $N_2$  obtained with  $s = 2.5 \cdot 10^{-9}$  cm. These values are, of course, considerably smaller than for  $N_2$  and  $s = 3 \cdot 10^{-9}$  cm, and not much larger than for  $O_2$  and  $s = 3 \cdot 10^{-9}$  cm. In the fifth row of Table VI A we have given  $\omega_0$  for  $N_2$  in air, assuming  $s = 2.5 \cdot 10^{-9}$  cm for the interaction  $N_2 - N_2$ ; the values thus obtained are only slightly less than those for  $O_2$  (first row).

On the other hand, if the first alternative explanation above is assumed, the interaction between two  $N_2$  molecules would have a large  $s$ , just as the interaction between two  $O_2$  molecules. In this case, the  $N_2 - N_2$  collisions would not contribute appreciably to the excitation of  $N_2$  vibrations, and  $\omega_0$  for  $N_2$  would be given by the third line in Table VI A in which the  $N_2 - O_2$  collisions alone are taken into account.

Finally, as a compromise, we have also given the results when  $s = 3 \cdot 10^{-9}$  cm is assumed to be valid for collisions between two  $N_2$  molecules as well as between  $N_2$  and  $O_2$  (fourth row of Table VI A).

The effect of water vapor on  $N_2$  is also unknown.  $H_2O$  is extremely effective in exciting the vibrations of  $O_2$  and  $CO_2$  (cf. Table V) as well as of  $N_{20}$ ,  $CS_2$  and  $COS$  (Knudsen and Fricke, loc. cit.). By pure analogy we might therefore

conclude that it would also be effective on  $H_2$ , and we have therefore included in Table IV a calculation of  $Z$  for collisions between  $H_2$  and  $H_2O$ , assuming the same  $s$  as for collisions between  $O_2$  and  $H_2O$  but taking into account the higher  $\gamma$  of  $H_2$ . However, it must be remembered that  $O_2$  has a chemical affinity to  $H_2O$  while  $H_2$  has very little; therefore, collisions with water may be much less effective on  $H_2$  ( $Z$  higher) than is indicated by the last line of Table IV.

In Table VI A, last row, we have computed  $\omega_0$  for collisions between  $H_2$  and  $H_2O$ , assuming 1 per cent water vapor in air of density  $1.18 \cdot 10^{-3}$ , and assuming the  $Z$  as given in Table IV. Presumably, these values of  $\omega_0$  are on the high side. Whether or not the humidity has an appreciable influence on the vibrations of  $H_2$ , depends not only on the temperature and on the correctness of our assumption about the interaction between  $H_2$  and  $H_2O$ , but also on the assumed interaction between  $H_2$  and  $H_2$ . If the latter is strong ( $s = 2.5 \cdot 10^{-9}$ ), the humidity is rather unimportant even at low  $T$ ; if it is weak (collisions with  $O_2$  only), the humidity is the decisive factor. This again indicates the extreme uncertainty of the data on the excitation of the vibration of  $H_2$ .

In Table VI B, we have calculated the mean free path for vibration,  $\lambda_v$ , on the high pressure side of a shock wave produced in "standard air", i.e., when the temperature and pressure on the low pressure side are  $300^\circ$  and 1 atmosphere respectively.  $\lambda_v$  is given in Table VI as a function of the temperature  $T_3$  which is obtained on the high pressure side at large distance from the front of the shock wave (par.3);  $T_3$  again is a known function of the velocity  $v_1$  of the shock wave (Table VIII). Velocity and density on the high pressure side were also taken from Table VIII (par.3), the asymptotic values  $v_3, \rho_3$  being used. The so defined  $\lambda_v$  is related to the  $\omega_0$  given in Table VI A by

$$\lambda_v = \frac{v_3}{\omega_0} \frac{\rho_1}{\rho_3} \quad (2.30)$$

Table VI. Relaxation Time and Mean Free Path of Vibration for  
 $O_2$  and  $N_2$  in Air.

Vibra-	Collisions with	Abun-	$s$	Temperature	300	500	700	1000	1500	2000	3000	5000
tion of	%	dance	( $10^{-9}$ cm)									
A. Reciprocal Relaxation Time $\omega_0$ (in $10^5$ sec $^{-1}$ )												
$O_2$	$N_2$	78	3	0.35	2.3	7	19	50	80	140	260	
	$H_2O$	1	0.93	1.1	2.8	5	7.5	11	13	14	17	
$N_2$	$O_2$	21	3	0.006	0.07	0.26	0.9	5.2	7	16	37	
	$N_2$	78	3	0.024	0.25	0.95	3.5	12	26	60	140	
	$N_2$	.78	2.5	0.10	0.9	3.0	9	30	55	115	240	
	$H_2O$	1	0.93	0.35	0.9	2.2	4	7	10	13	18	

		B. Mean Free Path of Vibration $\lambda_v$ (in millimeters)								
		$v_3 \cdot p_1 / p_3$ (meters/sec)	350	98	71	61	56	56	58	48
Vibra-	Collisions with									
$O_2$	$N_2$ only		10	0.43	0.10	0.032	0.011	0.007	0.004	0.0018
	$N_2$ and $H_2O$ (1%)		2.4	0.19	0.06	0.023	0.009	0.006	0.003 <sub>7</sub>	0.0017
$N_2$	$O_2$ only		550	14	2.7	0.7	0.18	0.08	0.03 <sub>6</sub>	0.013
	$O_2$ and $N_2$ ( $s=3 \cdot 10^{-9}$ cm)		110	3.0	0.6	0.14	0.03 <sub>7</sub>	0.017	0.007 <sub>5</sub>	0.0027
	$O_2$ and $N_2$ ( $s=2.5 \cdot 10^{-9}$ cm)		33	1.0	0.22	0.06	0.017	0.009	0.004 <sub>5</sub>	0.0017
	$O_2$ and 1% $H_2O$		10	1.0	0.20	0.12	0.05 <sub>5</sub>	0.033	0.020	0.009
	$O_2$ , $N_2$ ( $s=3 \cdot 10^{-9}$ ) and $H_2O$	9.5	0.8	0.21	0.07	0.025	0.013	0.006 <sub>5</sub>	0.0025	
	$O_2$ , $N_2$ ( $s=2.5 \cdot 10^{-9}$ )and $H_2O$	8	0.5	0.13	0.04	0.014	0.008	0.004	0.0016	

The quantity  $v_3 \cdot p_1/p_3$  is given in the first row of Table VI B, in meters per second. Then  $\lambda_v$  is given for various assumptions.

The value of  $\lambda_v$  for  $O_2$  in dry air decreases from 10 millimeters at 300° to 1/150 millimeter at 2000° and 1/500 at 5000°. If the initial pressure is low--let us say, 1/100 atmosphere-- $\lambda_v$  is proportionally greater (100 times) and may therefore easily reach considerable values. In wet air containing 1 per cent of water vapor by volume,  $\lambda_v$  for  $O_2$  is reduced to 2 mm at 300° but is almost the same as for dry air when  $T \geq 1500^\circ$  K.

For the vibrations of nitrogen, the value of  $\lambda_v$  is extremely uncertain. If the collisions with  $N_2$  are unimportant (cf. above) and if the air is dry, only collisions with  $O_2$  need to be considered; then  $\lambda_v$  is as large as half a meter at 300° K. Since the vibrational energy of  $N_2$  becomes important only for  $T > 600^\circ$  (Table III),  $\lambda_v$  is important only at higher temperatures; but even at  $T = 700^\circ$  we obtain  $\lambda_v \approx 3$  mm if only collisions with  $O_2$  are effective. On the other hand, if collisions with  $N_2$  are very effective ( $s = 2.5 \cdot 10^{-9}$  cm),  $\lambda_v$  is reduced by about a factor of 12 at 700°, and a factor of 8 at 5000°. If collisions with  $H_2O$  are as effective as assumed in Table IV and VI A, a water vapor content of 1 per cent reduces  $\lambda_v$  by factors varying from 9 to 1.05 when only temperatures  $\geq 700^\circ$  are considered.

Apart from the uncertainties in the assumptions, there is also an uncertainty in the Landau-Teller theory itself which makes the temperature dependence of  $\lambda_v$  uncertain by a factor of about 3 even if  $\omega_0$  at room temperature is accurately known.

The unsatisfactory state of our knowledge about the mean free path for molecular vibrations in air could be improved by experiments on the dispersion and absorption of sound in mixtures of  $O_2$  and  $N_2$  of varying composition and free from impurities. Such experiments should be done at  $T \geq 700^\circ$  K or higher in order to ensure sufficient excitation of the molecular vibrations of  $N_2$ . With such experiments available, the dependence of  $\lambda_v$  on the temperature at higher temperatures

could probably be calculated from the Landau-Teller theory with fair accuracy. The influence of humidity should also be investigated experimentally.

Nitrogen and oxygen are probably almost unique in their large values of  $Z$ , and therefore of  $\lambda_v$ . Other molecules have much lower frequencies or much greater chemical activity (cf. above). Therefore for most other gases, and especially for complicated polyatomic ones (explosives!),  $\lambda_v$  will in general be too small to be of any practical importance.

Dissociation. In Table VII, we give the number of molecular collisions  $Z_d$  required for one dissociation process, the reciprocal time of relaxation  $\omega_d$ , and the mean free path  $\lambda_d$  for dissociation. These quantities were calculated from Eqns. (2.28, 29 and 29a). The constants  $N$  and  $v$  were assumed as in Table VI, namely  $N = 5 \cdot 10^9$  sec<sup>-1</sup> at 300° K. and one atmosphere, and proportional to  $p\sqrt{T}$  otherwise;  $v$  equal to the velocity  $v_3$  of air on the high pressure side of a shock wave produced in "standard air";  $\alpha$  was taken from Table II,  $C_d$  was arbitrarily put equal to 1/100.  $Z_d$  is, of course, independent of the pressure;  $\omega_d$  is calculated for a density\* of  $1.18 \cdot 10^{-3}$  as in Table VI, and  $\lambda_d$  for the actual conditions on the high pressure side of a shock wave. It can be seen that the mean free paths obtained are very long indeed, decreasing for  $O_2$  from a little under one meter at 2500° to a little over one millimeter at 5000°. Therefore we should expect large effects from lack of dissociation equilibrium in shock waves which are sufficiently violent to produce dissociation. We must emphasize again the great uncertainty of the figures in Table VII which is caused by the lack of knowledge of  $C_d$ . Here again experiments would be desirable but they seem considerably more difficult than in the case of vibrations. Possibly studies of the dissociation equilibrium of other gases (e.g.,  $N_2 O_4$ ) would help.

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\* This is not quite consistent since  $\alpha$ , which occurs in (2.29), was calculated for an 8 times larger density, but  $p = 1.18 \cdot 10^{-3}$  was chosen for comparison with the  $\omega_o$  in Table VI.

Table VII. Relaxation Time and Mean Free Path for the Dissociation of Air

	T = 2500	3000	3500	4000	4500	5000
$\alpha$ {	0 <sub>2</sub> N <sub>2</sub>	0.00205 ----	0.0144 ----	0.0568 0.0003	0.152 0.0014	0.308 0.0051
$\lambda_o$ {	0 <sub>2</sub> N <sub>2</sub>	23.60 ----	19.67 ----	16.86 26.17	14.76 22.90	13.12 20.36
$Z_d$ {	0 <sub>2</sub> N <sub>2</sub>	7.5·10 <sup>10</sup> 9.2·10 <sup>11</sup>	1.85·10 <sup>9</sup> 4.0·10 <sup>10</sup>	1.27·10 <sup>8</sup> 3.5·10 <sup>9</sup>	1.76·10 <sup>7</sup> 5.1·10 <sup>8</sup>	3.8·10 <sup>6</sup> 5.1·10 <sup>8</sup>
$\omega_d$ { (sec <sup>-1</sup> )	0 <sub>2</sub> N <sub>2</sub>	85 -----	600 65	2400 320	6800 1080	16,600 2900
$v_3 \cdot P_1 / P_3$		57	58	57	55	52
$\lambda_d$ { (cm.)	0 <sub>2</sub> N <sub>2</sub>	670 -----	98 880	24 170	8.1 48	1.4 16

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**The Formation of Deuterons by Proton Combination**  
(with C. L. Critchfield)  
*Phys. Rev.* **54**, 248–254 (1938)

This is the fundamental nuclear reaction responsible for the energy of the sun. The idea was due to Charles Critchfield, and encouraged by George Gamow, his thesis adviser. I contributed mainly §3 and §4. At that, I left out the discussion of the nucleon spin: we have to start from two protons with opposite spin ( $^1S$  state) and end up with two nucleons with parallel spin ( $^3S$  state) in the deuteron. However, this is possible using Gamow-Teller selection rules. This deficiency was corrected in later papers by other authors.

The numerical result, in Table 2, seems rather low. The main change needed is the density at the center of the sun which should be closer to  $100g\ cm^{-3}$  than to  $10g\ cm^{-3}$ . A good discussion of modern theory is in J. N. Bahcall, *Neutrino Astrophysics* (Cambridge University Press, 1989), pp. 59–62.

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## The Formation of Deuterons by Proton Combination

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(Received June 23, 1938)

The probability of the astrophysically important reaction  $H + H = D + \epsilon^+$  is calculated. For the probability of positron emission, Fermi's theory is used. The penetration of the protons through their mutual potential barrier, and the transition probability to the deuteron state, can be calculated exactly, using the known interaction between two protons. The energy evolution due to the reaction is about 2 ergs per gram per second under the conditions prevailing at the center of the sun (density 80, hydrogen content 35 percent by weight, temperature  $2 \cdot 10^7$  degrees). This is almost but not quite sufficient to explain the observed average energy evolution of the sun (2 ergs/g sec.) because only a small part of the sun has high temperature and density. The reaction rate depends on the temperature approximately as  $T^{3.5}$  for temperatures around  $2 \cdot 10^7$  degrees.

### §1. INTRODUCTION

IT seems now generally accepted that the energy production in most stars is due to nuclear reactions involving light elements. Of all the elements, hydrogen is favored by its large abundance, by its large internal energy which makes a considerable energy evolution possible, and by its small charge and mass which enable it to penetrate easily through nuclear potential barriers. Again, of all reactions involving hydrogen, the most primitive is the combination of two protons to form a deuteron, with positron emission:



In fact, this reaction must stand in the beginning of any building up of chemical elements; it has already been discussed in this connection by v.

Weizsäcker.<sup>1</sup> However, there seems to be a general belief that reaction (1) is too rare to account for any appreciable fraction of the energy production in stars and that it can serve only to start the evolution of elements in a star which will then be carried on by other, more probable, processes. It is the purpose of this paper to show that this belief is unfounded but that reaction (1) gives an energy evolution of the correct order of magnitude for the sun.

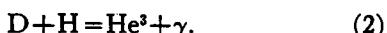
On the other hand, we do not want to imply that reaction (1) is the only important source of energy. An analysis of all possible nuclear reactions with light elements<sup>2</sup> shows that the capture of protons by carbon and nitrogen will also play an important role. It is more important

<sup>1</sup> V. Weizsäcker, Physik. Zeits. 38, 176 (1937).

<sup>2</sup> Bethe, to appear shortly in the Physical Review.

than (1) for heavy stars, less important for light ones and about equally important for the sun.

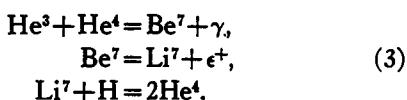
In calculating the energy evolution from reaction (1), it must be considered that (1) is followed by a number of other reactions which are all "fast" in comparison with (1) because they involve the emission of radiation or of heavy particles rather than of  $\beta$ -rays.<sup>3</sup> The deuterons formed in reaction (1) will first capture another proton, with  $\gamma$ -ray emission:



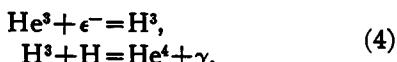
The ratio of the rates of reactions (2) and (1) is about  $10^{18}$  which means that, in equilibrium, there will be about one deuteron for  $10^{18}$  protons. This makes collisions between two deuterons very improbable and thus excludes any appreciable production of neutrons by such collisions.

The fate of the  $He^3$  formed in (2) depends to some extent on the question whether this nucleus or  $H^3$  is more stable. The most recent determination<sup>4</sup> of the energy evolution in the reaction  $H^2 + H^2 = He^3 + n^1$  seems to show that  $He^3$  is more stable while older determinations<sup>5</sup> gave the opposite result. The processes which occur are:

If  $He^3$  is more stable:



If  $H^3$  is more stable:



The net effect is in both cases the same, *viz.* the combination of four protons and two electrons to form an  $\alpha$ -particle. (The emission of a positron is equivalent to the consumption of an electron since the positron will ultimately annihilate an electron.) One  $\alpha$ -particle is formed for each process (1). The energy produced per process (1) is therefore equal to the difference in weight between four hydrogen atoms and one helium atom, *viz.* (cf. reference 5, 6)  $Q = 4 \cdot 1.008 13$

$$-4.003 86 = 0.028 66 \text{ mass units, i.e.,}$$

$$Q = 4.3 \cdot 10^{-5} \text{ erg.} \quad (5)$$

While the energy evolution in (3) and (4) is exactly the same, the processes lead to the formation of different intermediate products which could be of influence on the building up of heavier elements. However, it can be shown<sup>2</sup> that the building up of elements heavier than  $He^4$  is negligible under any circumstances so that the question of stability of  $He^3$  or  $H^3$  is actually not important.

In order to calculate the probability of the proton combination, the following factors have to be considered:

(1) The probability of collision of two protons which involves the penetrability of their mutual potential barrier. This can be calculated very accurately since the force between two protons is very well known from scattering experiments.<sup>7</sup>

(2) The probability of emission of a positron during the collision. This involves a theory of the  $\beta$ -decay. All available experimental evidence points to the conclusion that the original Fermi theory gives good agreement with the experimental dependence of lifetime on energy.

(3) The energy distribution of the protons in the star which is given by the Boltzmann law.

## §2. THE PROBABILITY OF POSITRON EMISSION

According to Fermi's theory, the probability of  $\beta$ -emission (per second) is

$$\beta = gf(W) |G|^2. \quad (6)$$

Here  $G$  is the matrix element of the nuclear transition,

$$G = \int \psi_i \psi_f d\tau, \quad (7)$$

$\psi_i$  and  $\psi_f$  the initial and final state of the nucleus, except for the substitution of one neutron by a proton.  $f$  is a function of the energy  $W$  of the emitted  $\beta$ -particle,

$$\begin{aligned} f(W) &= (W^2 - 1)^{\frac{1}{2}} \left( \frac{1}{30} W^4 - \frac{3}{20} W^2 - \frac{2}{15} \right) \\ &\quad + \frac{1}{4} W \log [W + (W^2 - 1)^{\frac{1}{2}}], \end{aligned} \quad (8)$$

<sup>3</sup> Cf. Bethe, Rev. Mod. Phys. 9, 188, § 76C (1937).

<sup>4</sup> Bonner, Phys. Rev. 53, 711 (1938).

<sup>5</sup> See Livingston and Bethe, Rev. Mod. Phys. 9, 373 (1937).

<sup>6</sup> Bainbridge, Phys. Rev. 53, 922A (1938).

<sup>7</sup> Tuve, Heydenburg and Hafstad, Phys. Rev. 50, 806 (1936).

where  $W$  is expressed in units of  $mc^2$  and includes the rest mass. A lower limit for the Fermi constant  $g$  can be deduced by assuming that  $G=1$  for transformations such as  $N^{13} \rightarrow C^{13} + e^+$ . This reaction has a half-life of 11.0 minutes and an upper limit of the  $\beta$ -spectrum (observed) of about 1.25 Mev, therefore  $\beta = \log 2/660 = 1.05 \cdot 10^{-3}$  sec. $^{-1}$ ,  $W=3.5$ ,  $f(W)=11.86$  and

$$g = 0.9 \cdot 10^{-4} \text{ sec.}^{-1}. \quad (9)$$

The (maximum) energy of the positron emitted in the combination of two protons follows from the very accurately known masses of proton and deuteron,<sup>5</sup> *viz.*:

$$\begin{aligned} \text{Two protons} &= 2 \cdot (1.00813 - 0.00055) = 2.01516 \\ \text{Deuteron} &= 2.01473 - 0.00055 = 2.01418 \end{aligned}$$

$$\begin{aligned} \text{Positron energy, including } mc^2 &= 0.00098 \\ (\text{mass units}), \text{ equivalent to } 1830 \cdot 0.00098 \text{ } mc^2 & \\ &= 1.80 \text{ } mc^2. \end{aligned}$$

For  $W=1.8$ , we have  $f(W)=0.132$  and therefore, with (6) and (9),

$$\beta = 1.2 \cdot 10^{-5} |G|^2 \text{ sec.}^{-1}. \quad (10)$$

A similar value is obtained by extrapolating the empirical Sargent curves to lower energy.  $\beta$  would be larger, if the matrix element  $G$  for the transformation  $N^{13} \rightarrow C^{13}$  is less than one. On the other hand, the Konopinski-Uhlenbeck theory would give about 10 times less for the decay constant. However, that theory seems to give too strong a dependence of decay constant on energy throughout, and will therefore not be used.

In calculating the matrix element  $G$  for the proton combination (1), it must be considered that the wave function of the deuteron is symmetric with respect to interchange of space and spin coordinates of proton and neutron while the wave function of two protons is antisymmetric.<sup>8</sup> In particular, when the two protons are in an  $S$  state (which is most favorable for their coming close together), their spins will be antiparallel (singlet) whereas the ground state of the deuteron is a triplet  $S$  state. The transition is therefore allowed only if the Gamow-Teller form<sup>9</sup> of the  $\beta$ -theory is used. This formulation permits a

change of direction of the spin of the proton which transforms into a neutron, and therefore a change of the total spin by one unit. Strong evidence for this theory is found<sup>10</sup> in the short life of  $He^6$ ; the  $\beta$ -transformation  $He^6 \rightarrow Li^6$  leads very probably from a  $^1S$  to a  $^3S$  state and is closely analogous to our process  $2H \rightarrow D$ . We shall therefore accept the Gamow-Teller theory in this paper. Moreover, we shall assume that the matrix element  $G$  in (10) can be calculated simply by integrating over the spatial coordinates of the two particles, i.e., that the summation over spins which is also implied in  $G$  gives unity. This assumption does not seem serious in view of the uncertainty in the numerical factor in (10).

If the original Fermi theory were taken instead of the Gamow-Teller theory, the transition  $H+H=D+e^+$  could occur only by virtue of the "small" components of the Fermi interaction, *viz.*  $\alpha_{\text{heavy particle}} \cdot \alpha_{\text{electron-neutrino}}$ . Since the Dirac operator  $\alpha_{\text{heavy}}$  (velocity) is "odd," its application on the  $^3S$  wave function of the deuteron ground state will give a function of  $^3P$  character. This can combine with the  $^3P$  part of the wave function of the incident protons. Due to the smallness of the latter and of the  $\alpha$ -operator itself, the transition probability will be greatly reduced, *viz.*, approximately by a factor

$$(W/I)^2(E/Mc^2) \approx 10^{-5},$$

where  $W=1.8 \text{ } mc^2$  is the energy evolution in the process,  $I=4.4 \text{ } mc^2$  the binding energy of the deuteron,  $E \approx 50 \text{ kev}$  the kinetic energy of the protons and  $Mc^2=931 \text{ Mev}$ . In this case, then, the energy evolution in the sun due to proton combination would be negligibly small.

### §3. THE COLLISION CROSS SECTION

According to the general principles of quantum theory, the cross section  $\sigma$  for the combination of two protons of relative velocity  $v$  is given by (6), (7) if we insert for  $\psi_i$  the wave function of two protons normalized to unit incident current. Thus we have

$$\sigma = gf(W)v^{-1} |\int \psi_p \psi_d d\tau|^2, \quad (11)$$

where  $\psi_d$  is the wave function of the ground state of the deuteron and  $\psi_p$  is normalized per unit

<sup>8</sup> We are indebted to Professor Oppenheimer for drawing our attention to this point.

<sup>9</sup> Gamow and Teller, Phys. Rev. 49, 895 (1936).

<sup>10</sup> Goldhaber, Phys. Rev. (to be published).

density at infinity. The integration goes over the space of the relative coordinates of the two protons (or proton and neutron, in the deuteron).

If we assume a square potential well of radius  $r_0$  and depth  $V_0$ , the normalized wave function of the deuteron is<sup>11</sup>

$$\psi_d = \begin{cases} (B/r) \exp(-(x-x_0)) & \text{for } r > r_0 \\ (B/r) \sin \mu x / \sin \mu x_0 & \text{for } r < r_0 \end{cases} \quad (12)$$

with the abbreviations

$$x = r/b, \quad x_0 = r_0/b, \quad (12a)$$

$$b = \hbar(M\epsilon)^{-\frac{1}{2}} = 4.37 \cdot 10^{-13} \text{ cm}, \quad (12b)$$

$$\mu = (V_0 - \epsilon/\epsilon)^{\frac{1}{2}}, \quad (12c)$$

$$B = (2\pi b)^{-\frac{1}{2}} (1+x_0)^{-\frac{1}{2}} (1+\mu^{-2})^{-\frac{1}{2}}. \quad (12d)$$

$M$  is the proton mass,  $\epsilon$  the binding energy of the deuteron, i.e., 2.17 Mev. Depth and width of the well are related by the condition

$$\mu \cot \mu x_0 = -1. \quad (12e)$$

The wave function of two protons, normalized to unit density, has the form  $e^{ikz}$  at large distances. (For considerations of symmetry, see §4.) It can be expanded in spherical harmonics and, at the small velocities prevailing in stars ( $\sim 10$  kilovolts), only the zero order term will be important. It has, at large distances, the form

$$\psi_p = \sin(\rho - \varphi)/\rho, \quad (13)$$

$$\text{where } \rho = kr, \quad k = Mv/2\hbar \quad (13a)$$

and  $\varphi$  is a phase (depending logarithmically on  $\rho$ ). At small distances, i.e., inside the nuclear potential well, we have

$$\psi_p = \frac{w}{r} = \frac{A}{r} \sin \frac{(MD)^{\frac{1}{2}}}{\hbar} r, \quad (14)$$

where  $D$  is the depth of the potential well between two protons, assumed "square" and of radius  $r_0$ ,  $A$  is a normalization factor. Outside of the well,  $\psi_p$  is a solution of the Schrödinger equation in the Coulomb field which may be written<sup>12</sup>

$$\psi_p = e^{ikr} \cos K(F + G \tan K)/kr. \quad (15)$$

Here  $F$  is the regular and  $G$  the irregular solution

of the Coulomb equation which behave asymptotically as  $\sin(\rho - \varphi_0)$  and  $\cos(\rho - \varphi_0)$ , respectively. As can be seen easily, (15) goes over asymptotically into (13).  $K$  is the phase shift due to the nuclear field, fixed by the condition of continuity of (14), (15) at  $r=r_0$ ; we have<sup>12</sup>

$$\tan K = F^2 \delta / [1 - FG\delta] \quad (16)$$

$$\text{with } \delta = \left( \frac{d \log F}{d\rho} - \frac{d \log w}{d\rho} \right)_{r_0}. \quad (16a)$$

For the small proton energies concerned,  $F(r_0)$  is very small (see below), both because of the Coulomb barrier and the small value of  $k$ . Therefore  $K$  will be very small ( $K=0.0017$  for  $v=e^2/\hbar$ , i.e. for a relative kinetic energy of 12.5 kev which gives the largest contribution to the cross section at a temperature of  $5 \cdot 10^7$  degrees) and  $e^{ikr} \cos K$  (cf. (15)) can be replaced by unity. Then the factor  $A$  in the internal wave function (14) is

$$A = \frac{F(r_0) + G(r_0) \tan K}{k \sin(MD)^{\frac{1}{2}} r_0 / \hbar}. \quad (17)$$

According to Yost, Wheeler and Breit,<sup>12</sup> the Coulomb wave functions may be written (for orbital momentum  $L=0$ )

$$F = C\rho\Phi, \quad G = C^{-1}\Theta, \quad (18)$$

where

$$C = (2\pi\eta)^{\frac{1}{2}} e^{-\pi\eta}, \quad \eta = e^2/\hbar v \quad (19)$$

contains the effect of the Coulomb barrier, and  $\Phi$  and  $\Theta$  are slowly varying functions of  $r$  which have the value 1 for  $r=0$ . Inserting into (16), (15) we get

$$\tan K = C^2 kr_0 \lambda, \quad (20)$$

$$\lambda = \Phi^2 \zeta / (1 - \Phi \Theta \zeta), \quad (20a)$$

$$\rho = \left( \frac{d \log F/w}{d \log \rho} \right)_{r_0} = \left( 1 + r \frac{d \log \Phi}{dr} - r \frac{d \log w}{dr} \right)_{r_0}, \quad (20b)$$

$$\psi_p = C[\Phi(r) + \lambda(r_0/r)\Theta(r)] \quad (r > r_0), \quad (21)$$

$$\psi_p = C \frac{r_0}{r} [\Phi(r_0) + \lambda\Theta(r_0)]$$

$$\times \frac{\sin \nu r/b}{\sin \nu r_0/b} \quad (r < r_0). \quad (22)$$

<sup>11</sup> Bethe and Bacher, Rev. Mod. Phys. 8, 110 (1936).

<sup>12</sup> Yost, Wheeler and Breit, Phys. Rev. 49, 174 (1936); J. Terr. Mag. 40, 443 (1935).

In the last expression, we have introduced the abbreviation

$$\nu = (MD)^{\frac{1}{2}} \hbar^{-1} b = (D/\epsilon)^{\frac{1}{2}}, \quad (22a)$$

which will be useful for the integration.  $\lambda$  represents the effect of the resonance due to the nuclear potential well.

For slow protons, the wave functions at small  $r$  are almost independent of the proton energy and have the form<sup>12</sup>

$$\begin{aligned} \Phi(y) &= y^{-\frac{1}{2}} I_1(2y^{\frac{1}{2}}) \\ &= 1 + \frac{y}{1!2!} + \frac{y^2}{2!3!} + \frac{y^3}{3!4!} + \dots, \end{aligned} \quad (23)$$

$$\Theta(y) = -2y^{\frac{1}{2}} K_1(2y^{\frac{1}{2}}) = 1 + y(\log y + 2\gamma - 1)\Phi - \sum_{s=1}^{\infty} \frac{y^{s+1}}{s!s+1!} \sum_{t=1}^s \left( \frac{1}{t} + \frac{1}{t+1} \right) \quad (23a)$$

with

$$\begin{aligned} y &= 2r/a, \quad a = 2\hbar^2/Mc^2 = 5.75 \cdot 10^{-12} \text{ cm}, \\ \gamma &= 0.577\dots \quad (\text{Euler's constant}). \end{aligned} \quad (23b)$$

The deviations from (23), (23a) for  $\eta=1$  are of the order of a percent.

Collecting our formulae, we may now write for the cross section (11)

$$\sigma = \frac{gf(W)}{v} \frac{(4\pi b^2)^2}{C^2} \frac{1}{2\pi b} \Lambda^2, \quad (24)$$

where

$$(1+x_0)^{\frac{1}{2}}(1+\mu^{-2})^{\frac{1}{2}}\Lambda = \Lambda_1 + \Lambda_2 + \Lambda_3, \quad (25)$$

$$\Lambda_1 = \frac{x_0[\Phi(r_0) + \lambda\Theta(r_0)]}{\sin \mu x_0 \sin \nu x_0} \int_0^{x_0} \sin \mu x \sin \nu x dx, \quad (25a)$$

$$\Lambda_2 = \int_{x_0}^{\infty} x dx \exp(-(x-x_0))\Phi(2bx/a), \quad (25b)$$

$$\Lambda_3 = \lambda x_0 \int_{x_0}^{\infty} dx \exp(-(x-x_0))\Theta(2bx/a). \quad (25c)$$

The integrations are elementary and give

$$\begin{aligned} \Lambda_1 &= \frac{\frac{1}{2}x_0^2[\Phi(r_0) + \lambda\Theta(r_0)]}{\sin \mu x_0 \sin \nu x_0} \\ &\times \left[ \frac{\sin(\mu-\nu)x_0}{(\mu-\nu)x_0} - \frac{\sin(\mu+\nu)x_0}{(\mu+\nu)x_0} \right], \end{aligned} \quad (26a)$$

$$\begin{aligned} \Lambda_2 &= 1 + x_0 + (2b/a)(1+x_0 + \frac{1}{2}x_0^2) \\ &+ \frac{1}{2}(2b/a)^2(1+x_0 + \frac{1}{2}x_0^2 + \frac{1}{6}x_0^3) + \dots, \end{aligned} \quad (26b)$$

$$\Lambda_3 = \lambda x_0 \{ 1 + (2b/a)[\log(2b/a) + 2\gamma - 1] \Lambda_2 \}$$

$$\begin{aligned} &- [(2b/a)^2 \frac{3}{2}(1+x_0 + \frac{1}{2}x_0^2) \\ &+ \frac{1}{2}(2b/a)^3 (7/3)(1+x_0 + \frac{1}{2}x_0^2 + \frac{1}{6}x_0^3)] \end{aligned}$$

$$+ \dots ] + \sum_{s=1}^{\infty} (2b/a)^s f_s(x_0)/(s-1)! \quad (26c)$$

with

$$f_s(x_0) = s!^{-1} \int_{x_0}^{\infty} \exp(-(x-x_0)) x^s \log x dx, \quad (26d)$$

$$f_1 = 1 + (1+x_0) \log x_0 - E_i(-x_0) \exp(x_0), \quad (26e)$$

$$\begin{aligned} f_2 &= \frac{3}{2} + \frac{1}{2}x_0 + (1+x_0 + \frac{1}{2}x_0^2) \log x_0 \\ &- E_i(-x_0) \exp(x_0), \end{aligned} \quad (26f)$$

$$\begin{aligned} f_3 &= (11/6) + (5/6)x_0 + \frac{1}{6}x_0^2 \\ &+ (1+x_0 + \frac{1}{2}x_0^2 + \frac{1}{6}x_0^3) \log x_0 \\ &- E_i(-x_0) \exp(x_0). \end{aligned} \quad (26g)$$

Table I gives the numerical results for two values of the radius  $r_0$  of the potential well, viz.  $e^2/mc^2$  and  $e^2/2 mc^2$ . The depth  $D$  of the proton-proton well was taken from Breit, Condon and Present.<sup>13</sup> All other quantities were calculated from the formulae in the text. It is seen that the contribution of the inside of the potential well,  $\Lambda_1$ , is rather small even for the larger  $r_0$ , which shows that the result will not depend sensitively on the shape of the potential well.

TABLE I. Numerical results for two values of the radius.

	$r_0 = e^2/mc^2$	$r_0 = e^2/2 mc^2$
$x_0$	0.645	0.322
$V_0$ (Mev)	20.9	66.5
$D$ (Mev)	10.3	47.0
$\mu$	2.94	5.45
$\nu$	2.18	4.65
$(rd \log w/dr)$	0.236	0.110
$\Phi(r_0)$	1.050	1.025
$\Theta(r_0)$	0.769	0.854
$(rd \log \Phi/dr)$	0.050	0.025
$\zeta$	0.814	0.915
$\lambda$	2.63	4.80
$\Lambda_1$	0.689	0.277
$\Lambda_2$	1.949	1.547
$\Lambda_3$	1.205	1.030
$(1+x_0)(1+\mu^{-2})$	1.835	1.367
$\Lambda$	2.84	2.44
$\Lambda^2$	8.08	5.93

<sup>13</sup> Breit, Condon and Present, Phys. Rev. 50, 825 (1936).

## FORMATION OF DEUTERONS

Furthermore, the contribution  $\Lambda_3$  which is due to resonance is smaller than  $\Lambda_2$ , which would be present even if there were only the Coulomb field between the two protons. The final result for  $\Lambda^2$  increases somewhat with increasing radius of the well. For  $\eta=1$ , a numerical calculation gave  $\Lambda^2=8.8$  instead of 8.1.

## §4. SYMMETRY, STATISTICS, ETC.

If  $N$  is the number of protons per  $\text{cm}^3$ , the probability of finding one proton with velocity  $\mathbf{v}_1$  and one with  $\mathbf{v}_2$ , is

$$N^2 \varphi(\mathbf{v}_1) \varphi(\mathbf{v}_2) d\mathbf{v}_1 d\mathbf{v}_2, \quad (27)$$

where  $\varphi$  is the Boltzmann distribution function. In calculating the total probability of our process, we must integrate over each pair of volume elements  $d\mathbf{v}_1 d\mathbf{v}_2$  only once; if we want to integrate over  $\mathbf{v}_1$  and  $\mathbf{v}_2$  independently, (27) must be divided by 2 (this corresponds to the fact that the total number of proton pairs is  $\frac{1}{2}N^2$ ). We can transform to relative velocity  $\mathbf{v} = \mathbf{v}_1 - \mathbf{v}_2$  and center-of-gravity velocity  $\mathbf{V} = \frac{1}{2}(\mathbf{v}_1 + \mathbf{v}_2)$  and integrate over the latter, then we obtain (including the factor  $\frac{1}{2}$  mentioned)

$$\frac{1}{2} N^2 \varphi(\mathbf{v}) d\mathbf{v} \quad (27a)$$

$$\varphi(\mathbf{v}) d\mathbf{v} = (M/4\pi kT)^{\frac{3}{2}} \times \exp(-Mv^2/4kT) 4\pi v^2 dv. \quad (28)$$

Of the proton pairs with given velocities  $\mathbf{v}_1 \mathbf{v}_2$ , one in four will have opposite spins, three in four parallel spins. The latter have an anti-symmetrical spatial wave function and therefore do not contribute to the cross section of our nuclear process. The former have a symmetrical wave function which is, normalized to unit density:

$$[(\exp(i\mathbf{k}_1 \cdot \mathbf{r}_1 + i\mathbf{k}_2 \cdot \mathbf{r}_2)) + (\exp(i\mathbf{k}_2 \cdot \mathbf{r}_1 + i\mathbf{k}_1 \cdot \mathbf{r}_2))] / \sqrt{2}. \quad (29)$$

Separating off the motion of the center of gravity and expanding into spherical harmonics, we obtain

$$(\exp(ikz) + \exp(-ikz)) / \sqrt{2} = \sqrt{2} \sin kr / kr + \dots, \quad (29a)$$

which differs from (13) by a factor of  $\sqrt{2}$ . This gives a factor 2 in the cross section and, with the

TABLE II. Energy evolution due to proton combination, for  $\rho c_H^2 = 10 \text{ g/cm}^3$ .

$r$ (million degrees)	5	10	15	20	30	40	50	70	100
$\tau$ (ergs/g sec.)	19.8 0.0040	15.70 0.15	13.72 0.76	12.56 2.2	10.89 9.1	9.90 20	9.18 36	7.28 150	

factor  $\frac{1}{4}$  for the *a priori* probability of opposite spin, there remains a factor  $\frac{1}{2}$ .

The total number of processes per  $\text{cm}^3$  per sec. becomes thus

$$p' = \frac{1}{4} N^2 \int \varphi(\mathbf{v}) d\mathbf{v} v \sigma. \quad (30)$$

By the insertion of (24), (28), (19), this becomes

$$p' = \pi^{\frac{1}{2}} g f(W) N^2 b^3 \Lambda^2 \left( \frac{M}{kT} \right)^{\frac{1}{2}} \int_0^\infty v^2 dv \times \frac{2\pi e^2}{\hbar v} \exp \left( -\frac{2\pi e^2}{\hbar v} - \frac{Mv^2}{4kT} \right). \quad (31)$$

The integrand has a strong maximum very close to

$$v = (4\pi e^2 kT / \hbar M)^{\frac{1}{2}}. \quad (31a)$$

Approximating it, in the usual way, by a Gaussian around the maximum, we find

$$p' = 16\pi \cdot 3^{-\frac{1}{2}} \cdot g f(W) N^2 b^3 \Lambda^2 r^2 e^{-r} \quad (32)$$

with

$$r = 3(\pi^2 M e^4 / 4\hbar^2 k T)^{\frac{1}{2}}. \quad (33)$$

If  $t$  is the temperature in millions of degrees, we have

$$r = 33.8 t^{-\frac{1}{2}}. \quad (33a)$$

## §5. RESULT

We insert into (32) the values of the constants  $b$  (cf. (12b)),  $g f(W)$  from (10),  $\Lambda^2$  from Table I (for  $r_0 = e^2/mc^2$ ), and assume that the concentration of hydrogen (by weight) is  $c_H$  and the density (in  $\text{g/cm}^3$ ) is  $\rho$ . Then the number of processes per gram per second is

$$p = p'/\rho = 16\pi \cdot 3^{-\frac{1}{2}} \cdot 1.2 \cdot 10^{-5} \cdot (6.02 \cdot 10^{23})^2 \cdot (4.37 \cdot 10^{-13})^3 \cdot 8.10 \cdot \rho c_H^2 r^2 e^{-r} = 0.95 \cdot 10^7 \rho c_H^2 r^2 e^{-r}. \quad (34)$$

Each combination of two protons leads (§1) ultimately to the formation of an  $\alpha$ -particle out of four protons and two electrons, with an energy liberation of  $4.3 \cdot 10^{-5}$  erg. Therefore the

energy production is

$$\epsilon = 410 \rho c_H^2 r^2 e^{-r} \text{ ergs/gram sec.} \quad (35)$$

The density at the center of the sun<sup>14</sup> is about 80, the hydrogen content  $c_H \approx 0.35$ , therefore  $\rho c_H^2 \sim 10$ . Table II gives the energy evolution due to the proton-proton reaction at various temperatures. With a hydrogen content of 35 percent, the central temperature of the sun is about  $20 \cdot 10^6$  degrees. At this temperature, the energy production is about 2.2 ergs/g sec. This is of the same order as the observed average energy production of the sun (2.0 ergs/g sec.). Thus we come to the conclusion that the *proton-proton combination gives an energy evolution of the right order of magnitude for the sun.*

For a quantitative comparison, it must be remembered that both the temperature and the density of the sun decrease fairly rapidly from the center outwards, and that the rate of reaction decreases with both of these quantities. The average energy production per gram will

<sup>14</sup> Stromgren, *Ergebn. d. exakt. Naturwiss.* **16**, (1937).

thus be considerably smaller than that at the center, perhaps by a factor of 10. Since our calculations are rather accurate, it seems that there must be another process contributing somewhat more to the energy evolution in the sun. This is probably the capture of protons by carbon (reference 2).

For many problems, it is necessary to know the temperature dependence of the energy production  $\epsilon$ . It is convenient to express this dependence as a power law,  $\epsilon \sim T^n$ . Then (cf. (35))

$$n = d \log \epsilon / d \log T = \frac{1}{3}(\tau - 2). \quad (36)$$

At 20 million degrees, this gives in our case  $n = 3.5$ . This is large enough to make the point source model of stars a rather good approximation. On the other hand, it is too slow a dependence on temperature to explain, with temperatures of the order  $2-4 \cdot 10^7$  degrees, the very high rates of energy production found in very heavy stars. However, we believe that our process is the principal source of energy in stars lighter than the sun.

## Energy Production in Stars

*Phys. Rev.* **55**, 434–456 (1939)

The main point is the discovery and calculation of the carbon-nitrogen cycle which powers main sequence stars heavier than the sun. It was mainly for this paper that I received the Nobel Prize for Physics in 1967. The paper originated from a small conference in Washington, March 1938, sponsored jointly by the George Washington University and the Carnegie Institution. The conference was concerned with energy production in stars. The direct combination of two protons (see previous paper) had been established as a satisfactory energy source for the sun, but could not explain the enormous increase of luminosity with increasing mass of the star. From Eddington's theory of the internal constitution of stars, it was known that the central temperature increases only slowly with the mass of the star. It was therefore necessary to find nuclear reactions depending more strongly on temperature than  $H + H$ , pointing to the involvement of heavier nuclei than  $H$ . At the same time, it was known that the abundance of heavier nuclei is much smaller than that of hydrogen. The CN cycle fits both requirements: it involves the heavier nuclei, C and N, but they are regenerated in the cycle, only the abundant H is consumed.

The CN cycle is now generally accepted by astrophysicists as the source of energy of the heavier stars in the main sequence. The nuclear reactions involved have been measured by W. A. Fowler and his collaborators at Caltech, and the resulting energy production agrees well with that calculated in this paper. Further confirmation comes from the observation that near a number of heavy stars there are clouds in which N is highly enriched relative to C and O, compared with the average in the galaxy. (Oxygen is transformed, by a slower reaction, into C and N): this is to be expected from the CN cycle since  $^{14}\text{N}$  has a longer life than  $^{12}\text{C}$ .

In modern computations of stellar evolution, the CN cycle is assumed as a basis.

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## Energy Production in Stars\*

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It is shown that the most important source of energy in ordinary stars is the reactions of carbon and nitrogen with protons. These reactions form a cycle in which the original nucleus is reproduced, *viz.*  $C^{12} + H = N^{13}$ ,  $N^{13} = C^{12} + e^+$ ,  $C^{12} + H = N^{14}$ ,  $N^{14} + H = O^{15}$ ,  $O^{15} = N^{15} + e^+$ ,  $N^{15} + H = C^{12} + He^4$ . Thus carbon and nitrogen merely serve as catalysts for the combination of four protons (and two electrons) into an  $\alpha$ -particle (§7).

The carbon-nitrogen reactions are unique in their cyclical character (§8). For all nuclei lighter than carbon, reaction with protons will lead to the emission of an  $\alpha$ -particle so that the original nucleus is permanently destroyed. For all nuclei heavier than fluorine, only radiative capture of the protons occurs, also destroying the original nucleus. Oxygen and fluorine reactions mostly lead back to nitrogen. Besides, these heavier nuclei react much more slowly than C and N and are therefore unimportant for the energy production.

The agreement of the carbon-nitrogen reactions with observational data (§7, 9) is excellent. In order to give the correct energy evolution in the sun, the central temperature of the sun would have to be 18.5 million degrees while

integration of the Eddington equations gives 19. For the brilliant star Y Cygni the corresponding figures are 30 and 32. This good agreement holds for all bright stars of the main sequence, but, of course, not for giants.

For fainter stars, with lower central temperatures, the reaction  $H + H = D + e^+$  and the reactions following it, are believed to be mainly responsible for the energy production. (§10)

It is shown further (§5-6) that no elements heavier than  $He^4$  can be built up in ordinary stars. This is due to the fact, mentioned above, that all elements up to boron are disintegrated by proton bombardment ( $\alpha$ -emission!) rather than built up (by radiative capture). The instability of  $Be^8$  reduces the formation of heavier elements still further. The production of neutrons in stars is likewise negligible. The heavier elements found in stars must therefore have existed already when the star was formed.

Finally, the suggested mechanism of energy production is used to draw conclusions about astrophysical problems, such as the mass-luminosity relation (§10), the stability against temperature changes (§11), and stellar evolution (§12).

## §1. INTRODUCTION

THE progress of nuclear physics in the last few years makes it possible to decide rather definitely which processes can and which cannot occur in the interior of stars. Such decisions will be attempted in the present paper, the discussion being restricted primarily to main sequence stars. The results will be at variance with some current hypotheses.

The first main result is that, under present conditions, no elements heavier than helium can be built up to any appreciable extent. Therefore we must assume that the heavier elements were built up before the stars reached their present state of temperature and density. No attempt will be made at speculations about this previous state of stellar matter.

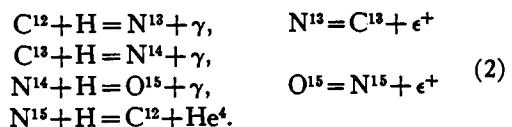
The energy production of stars is then due entirely to the combination of four protons and two electrons into an  $\alpha$ -particle. This simplifies the discussion of stellar evolution inasmuch as

the amount of heavy matter, and therefore the opacity, does not change with time.

The combination of four protons and two electrons can occur essentially only in two ways. The first mechanism starts with the combination of two protons to form a deuteron with positron emission, *viz.*



The deuteron is then transformed into  $He^4$  by further capture of protons; these captures occur very rapidly compared with process (1). The second mechanism uses carbon and nitrogen as catalysts, according to the chain reaction



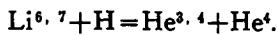
The catalyst  $C^{12}$  is reproduced in all cases except about one in 10,000, therefore the abundance of carbon and nitrogen remains practically unchanged (in comparison with the change of the number of protons). The two reactions (1) and

\* Awarded an A. Cressy Morrison Prize in 1938, by the New York Academy of Sciences.

(2) are about equally probable at a temperature of  $16 \cdot 10^6$  degrees which is close to the central temperature of the sun ( $19 \cdot 10^6$  degrees<sup>1</sup>). At lower temperatures (1) will predominate, at higher temperatures, (2).

No reaction other than (1) or (2) will give an appreciable contribution to the energy production at temperatures around  $20 \cdot 10^6$  degrees such as are found in the interior of ordinary stars. The lighter elements (Li, Be, B) would "burn" in a very short time and are not replaced as is carbon in the cycle (2), whereas the heavier elements (O, F, etc.) react too slowly. Helium, which is abundant, does not react with protons because the product, Li<sup>5</sup>, does not exist; in fact, the energy evolution in stars can be used as a strong additional argument against the existence of He<sup>5</sup> and Li<sup>5</sup> (§3).

Reaction (2) is sufficient to explain the energy production in very luminous stars of the main sequence as Y Cygni (although there are difficulties because of the quick exhaustion of the energy supply in such stars which would occur on any theory, §9). Neither of the reactions (1) or (2) is capable of accounting for the energy production in giants; if nuclear reactions are at all responsible for the energy production in these stars it seems that the only ones which could give sufficient energy are



It seems, however, doubtful whether the energy production in giants is due to nuclear reactions at all.<sup>2</sup>

We shall first calculate the energy production by nuclear reactions (§2, 4). Then we shall prove the impossibility of building up heavier elements under existing conditions (§5–6). Next we shall discuss the reactions available for energy production (§5, 7) and the results will be compared with available material on stellar temperatures and densities (§8, 9). Finally, we shall discuss the astrophysical problems of the mass-luminosity relation (§10), the stability of stars against temperature changes (§11) and stellar evolution (§12).

<sup>1</sup> B. Strömgren, *Ergebn. d. Exakt. Naturwiss.* **16**, 465 (1937).

<sup>2</sup> G. Gamow, private communication.

## §2. FORMULA FOR ENERGY PRODUCTION

The probability of a nuclear reaction in a gas with a Maxwellian velocity distribution was first calculated by Atkinson and Houtermans.<sup>3</sup> Recently, an improved formula was derived by Gamow and Teller.<sup>4</sup> The total number of processes per gram per second is<sup>4</sup>

$$p = \frac{4}{3^{5/2}} \frac{\rho x_1 x_2 \Gamma}{m_1 m_2 \hbar} a R^2 e^{-(2R/a)^{1/2}} \tau^2 e^{-\tau}. \quad (4)$$

Here  $\rho$  is the density of the gas,  $x_1 x_2$  the concentrations (by weight) of the two reacting types of nuclei,  $m_1 m_2$  their masses,  $Z_1 e$  and  $Z_2 e$  their charges,  $m = m_1 m_2 / (m_1 + m_2)$  the reduced mass,  $R$  the combined radius,

$$a = \hbar^2 / me^2 Z_1 Z_2, \quad (5)$$

the "Bohr radius" for the system,  $\Gamma/\hbar$  the probability of the nuclear reaction, in sec.<sup>-1</sup>, after penetration, and

$$\tau = 3 \left( \frac{\pi^2 m e^4 Z_1^2 Z_2^2}{2 \hbar^2 k T} \right)^{1/2}. \quad (6)$$

If we measure  $\rho$  in g/cm<sup>3</sup>,  $\Gamma$  in volts and  $T$  in units of  $10^6$  degrees, we have

$$p = 5.3 \cdot 10^{25} \rho x_1 x_2 \Gamma \varphi (Z_1, Z_2) \tau^2 e^{-\tau} \text{ g}^{-1} \text{ sec.}^{-1}, \quad (7)$$

$$\tau = 42.7 (Z_1 Z_2)^{1/2} (A/T)^{1/4}, \quad (8)$$

$$\varphi = \frac{1}{A_1 A_2 (Z_1 Z_2 A)^{1/2}} \left( \frac{8R}{a} \right)^2 e^{-(8R/a)^{1/2}}, \quad (9)$$

where  $A_1 A_2$  are the atomic weights of the reacting nuclei ( $A_i = m_i/m_H$ ),  $A = m/m_H$ ,  $m_H$  = mass of hydrogen. For the combined radius of nuclei 1 and 2 we put

$$R = 1.6 \cdot 10^{-13} (A_1 + A_2)^{1/2} \text{ cm.} \quad (10)$$

Then we obtain for  $\varphi$  the values given in Table I. The values of  $\varphi$  for isotopes of the same element differ only very slightly.

The values of  $\Gamma$  for reactions giving particles can be deduced from the *observed* cross sections

<sup>3</sup> R. d'E. Atkinson and F. G. Houtermans, *Zeits. f. Physik* **54**, 656 (1929).

<sup>4</sup> G. Gamow and E. Teller, *Phys. Rev.* **53**, 608 (1938), Eq. (3).

TABLE I. Values of  $\varphi$  for various nuclear reactions.

REACTION	$R$ ( $10^{-15}$ CM)	$\varphi$	REACTION	$R$	$\varphi$
$H^2+H$	2.3	0.38	$Si^{30}+H$	5.0	29.3
$H^3+H$	2.5 <sub>s</sub>	0.48	$Cl^{37}+H$	5.4	75
$He^4+H$	2.7 <sub>s</sub>	0.81	$H^2+H^2$	2.5 <sub>s</sub>	0.67
$Li^7+H$	3.2	0.91	$Be^7+H^2$	3.3	1.18
$Be^9+H$	3.4 <sub>s</sub>	1.16	$Be^7+He^3$	3.4 <sub>s</sub>	7.9
$B^{11}+H$	3.6 <sub>s</sub>	1.52	$He^4+H^2$	2.9	0.57
$C^{12}+H$	3.7 <sub>s</sub>	2.00	$He^4+He^3$	3.0 <sub>s</sub>	1.09
$N^{14}+H$	3.9 <sub>s</sub>	2.78	$He^4+He^4$	3.2	1.29
$O^{16}+H$	4.1	3.80	$Li^7+He^4$	3.5 <sub>s</sub>	4.9
$F^{19}+H$	4.3 <sub>s</sub>	5.5	$Be^7+He^4$	3.5 <sub>s</sub>	13.2
$Ne^{20}+H$	4.5 <sub>s</sub>	7.7	$Be^9+He^4$	3.6 <sub>s</sub>	16.2
$Mg^{26}+H$	4.8	13.2	$C^{12}+He^4$	4.0	230

TABLE II. Cross sections and widths for some nuclear reactions giving particles.

REACTION	REF.	E KV	$\sigma$ CM <sup>2</sup>	R CM	$\Gamma$
$H^2+H^2 = He^4+n^1$	5	100	$1.7 \cdot 10^{-26}$	$2.6 \cdot 10^{-13}$	$3 \cdot 10^5$
$Li^7+H^1 = 2He^4$	6	42	$1.7 \cdot 10^{-26}$	$3.2 \cdot 10^{-13}$	$4 \cdot 10^4$
$Li^6+H^1 = He^4+He^3$	yield ~ same as $Li^7+H$ in natural $Li$				$5 \cdot 10^5$
$target$					
$Li^6+H^2 = [2He^4]$	7	212	$1.9 \cdot 10^{-26}$	$3.2 \cdot 10^{-13}$	$4 \cdot 10^4$
$Li^7+H^2 = [2He^4+n^1]$	7	212	$5.5 \cdot 10^{-26}$	$3.3 \cdot 10^{-13}$	$10^7$
$Be^9+H^1 = [Li^7+H^1]$	7a	212	$1.1 \cdot 10^{-25}$	$3.5 \cdot 10^{-13}$	$1.7 \cdot 10^7$
$Be^9+H^2 = [Be^9+H^2]$	7a	212	$5 \cdot 10^{-26}$	$3.6 \cdot 10^{-13}$	$6 \cdot 10^6$
$Be^9+H^2 = [Be^9+H^1]$	7b	212	$6 \cdot 10^{-26}$	$3.7 \cdot 10^{-13}$	$2 \cdot 10^6$

of such reactions with the use of the formula (cf. reference 4, Eq. (2))

$$\sigma = \frac{\pi R^2}{2E} \frac{A_1 + A_2}{A_2} \Gamma \exp \left[ \left( \frac{32R}{a} \right)^{\frac{1}{2}} - \frac{2\pi e^2}{\hbar v} Z_1 Z_2 \right] \quad (11)$$

where  $E$  is the absolute energy of the incident particle (particle 1). Table II gives the experimental results for some of the better investigated reactions. In each case, experiments with low energy particles were chosen in order to make the conditions as similar as possible to those in stars where the greatest number of nuclear reactions is due to particles of about 20 kilovolts energy. The cross sections were in each case calculated from the thick target yield with the help of the range-energy relation of Herb,

<sup>5</sup> R. Ladenburg and M. H. Kanner, Phys. Rev. 52, 911 (1937).

<sup>6</sup> H. D. Doolittle, Phys. Rev. 49, 779 (1936).

<sup>7</sup> J. H. Williams, W. G. Shepherd and R. O. Haxby, Phys. Rev. 52, 390 (1937).

<sup>7a</sup> J. H. Williams, R. O. Haxby and W. G. Shepherd, Phys. Rev. 52, 1031 (1937).

<sup>7b</sup> J. H. Williams, W. H. Wells, J. T. Tate and E. J. Hill, Phys. Rev. 51, 434 (1937).

Bellamy, Parkinson and Hudson.<sup>8</sup> The widths obtained (last column of Table II) are mostly between  $3 \cdot 10^5$  and  $2 \cdot 10^7$  ev, with the exception of the reaction  $Li^7+H = 2He^4$  which is known to be "improbable."<sup>9</sup>

The  $\gamma$ -ray widths  $\Gamma_\gamma$  can be obtained from observed resonance capture of protons. Table III gives the experimental results. Two of the older data were taken from Table XXXIX of reference 10; all the others are from more recent experiments on proton<sup>11-14</sup> and neutron<sup>15</sup> capture. Although the results of different investigators differ considerably (e.g., for  $Li^7+H^1 = Be^8$ ,  $\Gamma$  is between 4 and 40 volts the latter value being more likely) they seem to lie generally between about  $\frac{1}{2}$  and 40 volts. Ordinarily, the width is somewhat larger for the more energetic  $\gamma$ -rays, as is expected theoretically. A not too bad approximation to the experiments is obtained by using the theoretical formula for dipole radiation (reference 10, Eq. (711b)) with an oscillator strength of 1/50. This gives

$$\Gamma_\gamma \sim 0.1 E_\gamma^2, \quad (12)$$

TABLE III.  $\gamma$ -ray widths of nuclear levels.

REACTION	REFERENCE	WIDTH (VOLTS)	$\gamma$ -RAY ENERGY (MEV)
$Li^7+H^1 = Be^8+\gamma$	{ 10 11	{ 4 40	17
$B^{11}+H^1 = C^{12}+\gamma$	11	0.6	12, 16
$C^{12}+H^1 = N^{13}+\gamma$	12	0.6	2
$C^{12}+H^1 = N^{14}+\gamma$	13, 14	30	4, 8
$F^{19}+H^1 = Ne^{20}+\gamma$	10	0.6, 8, 18	6
$C^{12}+n^1 = C^{13}+\gamma$	15	<2.5	5
$O^{16}+n^1 = O^{17}+\gamma$	15	<2.5	4

<sup>8</sup> D. B. Parkinson, R. G. Herb, J. C. Bellamy and C. M. Hudson, Phys. Rev. 52, 75 (1937).

<sup>9</sup> M. Goldhaber, Proc. Camb. Phil. Soc. 30, 560 (1934).

<sup>10</sup> H. A. Bethe, Rev. Mod. Phys. 9, 71 (1937).

<sup>11</sup> W. A. Fowler, E. R. Gaerttner and C. C. Lauritsen, Phys. Rev. 53, 628 (1938).

<sup>12</sup> R. B. Roberts and N. P. Heydenburg, Phys. Rev. 53, 374 (1938).

<sup>13</sup> P. I. Dee, S. C. Curran and V. Petříčka, Nature 141, 642 (1938). The  $\gamma$ -rays from  $C^{13}$  give about equally as many counts as those from  $C^{12}$ . The efficiency of the counter for  $C^{13}$   $\gamma$ -rays is about twice that for  $C^{12}$ , because the cross section for production of Compton and pair electrons is smaller by a factor 2/3 while the range of these electrons is about 3 times longer. With an abundance of  $C^{13}$  of about 1 percent, the  $\gamma$ -width for this nucleus becomes 50 times that of  $C^{12}$ . I am indebted to Dr. Rose for these calculations.

<sup>14</sup> M. E. Rose, Phys. Rev. 53, 844 (1938).

<sup>15</sup> O. R. Frisch, H. v. Halban and J. Koch, Nature 140 895 (1937); Danish Acad. Sci. 15, 10 (1937).

where  $E_\gamma$  is the  $\gamma$ -ray energy in mMU (milli-mass-units), and  $\Gamma_\gamma$  the  $\gamma$ -ray width in volts. For quadrupole radiation, theory gives about

$$\Gamma_\gamma \sim 5 \cdot 10^{-4} E_\gamma^4 \quad (\text{quadrupole}). \quad (12a)$$

Formulae (12), and (12a) will be used in the calculations where experimental data are not available; they may, in any individual case, be in error by a factor 10 or more but such a factor is not of great importance compared with other uncertainties.

It should be noted that quite generally radiative processes are rare compared with particle emission. According to the figures given in Tables II and III, the ratio of probabilities is  $10^4\text{--}10^5$  in favor of particle reactions.

In a number of cases, the reaction of a nucleus  $A$  with a heavy particle (proton, alpha-) must compete with natural  $\beta$ -radioactivity of  $A$  or with electron capture. In those cases where the lifetime of radioactive nuclei is not known experimentally, we use the Fermi theory. According to this theory, the decay constant for  $\beta$ -emission is<sup>16</sup>

$$\beta = 0.9 \cdot 10^{-4} f(W) |G|^2 \text{ sec.}^{-1}. \quad (13)$$

The matrix element  $G$  is about unity for strongly allowed transitions, and

$$f(W) = (W^2 - 1)^{\frac{1}{2}} \left( \frac{1}{30} W^4 - \frac{3}{20} W^2 - \frac{2}{15} \right) + \frac{1}{4} W \log \{W + (W^2 - 1)^{\frac{1}{2}}\}, \quad (13a)$$

where  $W$  is the maximum energy of the  $\beta$ -particle, including its rest mass, in units of  $mc^2$  ( $m$ =electron mass).

The probability of electron capture is

$$\beta_C = 0.9 \cdot 10^{-4} \pi^2 N (\hbar/mc)^3 W^2 |G|^2 \text{ sec.}^{-1}, \quad (14)$$

where  $W$  is the energy of the emitted neutrino in units of  $mc^2$  and  $N$  the number of electrons per unit volume. If the hydrogen concentration is  $x_H$ , we have (reference 1, p. 482)  $N = 6 \cdot 10^{23} \rho \cdot \frac{1}{2} (1+x_H)$  ( $\rho$  the density), and

$$\beta_C = 1.5 \cdot 10^{-11} \rho (1+x_H) W^2 |G|^2 \text{ sec.}^{-1}. \quad (14a)$$

<sup>16</sup> C. L. Critchfield and H. A. Bethe, Phys. Rev. 54, 248, 862 (L) (1938).

### §3. STABILITY OF UNKNOWN ISOTOPES

For the discussion of nuclear reactions it is essential to know whether or not certain isotopes exist (such as Li<sup>4</sup>, Li<sup>5</sup>, Be<sup>6</sup>, Be<sup>8</sup>, B<sup>8</sup>, B<sup>9</sup>, C<sup>10</sup>, etc.). The criterion for the existence of a nucleus is its energetic stability against spontaneous disintegration into heavy particles (emission of a neutron, proton or alpha-particle). Whenever a light nucleus is energetically unstable against heavy particle emission, its life will be a very small fraction of a second (usually  $\sim 10^{-20}$  sec.) even if the instability is slight (e.g., Be<sup>8</sup> will have a life of  $10^{-13}$  sec. if it is by 50 kv heavier than two  $\alpha$ -particles<sup>17</sup>).

For the question of the lifetime of radioactive nuclei, it is also necessary to know the mass difference between isobars. Similar information is required for estimating the  $\gamma$ -ray width in capture reactions (cf. Eqs. (12), (12a)).

#### H<sup>3</sup> and He<sup>3</sup>

The most recent determination<sup>18</sup> of the reaction energy in the reaction  $H^2 + H^2 = He^3 + n^1$  yielded 3.29 Mev as compared with 3.98 in  $H^2 + H^2 = H^3 + H^1$ . With a mass difference of 0.75 Mev between neutron and hydrogen atom,<sup>19</sup> this makes He<sup>3</sup> more stable than H<sup>3</sup> by 0.06 Mev. This would be in agreement with the experimental fact that no H<sup>3</sup> is present in natural hydrogen to more than 1 part in  $10^{12}$ . Even if He<sup>3</sup> should turn out to be heavier than H<sup>3</sup>, the difference cannot be greater than about 0.05 Mev =  $0.1 mc^2$  which would make the life of He<sup>3</sup> exceedingly long ( $\sim 2000$  years at the center of the sun, (Eq. (14a)), 3000 years in the complete atom, on earth).

#### H<sup>4</sup> and Li<sup>4</sup>

As was first pointed out by Bothe and Gentner,<sup>20</sup> it is definitely possible that H<sup>4</sup> is stable. Li<sup>4</sup> is, of course, less stable because of the Coulomb repulsion between its three protons. If it is stable, Li<sup>4</sup> would be formed when He<sup>3</sup> captures a proton and would thus play an important role in stars (cf. §5). The only possible estimate of the stability seems to be a comparison

<sup>17</sup> H. A. Bethe, Rev. Mod. Phys. 9, 167 (1937).

<sup>18</sup> T. W. Bonner, Phys. Rev. 52, 685 (1938).

<sup>19</sup> H. A. Bethe, Phys. Rev. 53, 313 (1938).

<sup>20</sup> W. Bothe and W. Gentner, Naturwiss. 24, 17 (1936).

of  $\text{Li}^4\text{Li}^5$  to the analogous pair  $\text{B}^8\text{B}^9$ . Reasonable estimates<sup>21</sup> make  $\text{B}^9$  just unstable (0.3–0.7 mMU), while  $\text{B}^8$  comes out at the limit of stability (binding energy between –0.4 and +0.4 mMU), i.e.,  $\text{B}^8$  about 0.3 to 0.7 mMU more stable than  $\text{B}^9$ .  $\text{Li}^5$  (see below) is unstable by 1.4–1.8 mMU; if one assumes the same difference,  $\text{Li}^4$  is found to be unstable by ~1 mMU. However, this argument is very uncertain and the possibility of a stable  $\text{Li}^4$  cannot be excluded at present.  $\text{H}^4$  would, from a similar argument, turn out stable by 0.6 mMU.

### $\text{He}^5$ and $\text{Li}^5$

The instability of  $\text{He}^5$  is shown directly by the experiments of Williams, Shepherd and Haxby<sup>22</sup> on the reaction



From a measurement of the range of the  $\alpha$ -particles, the mass of  $\text{He}^5$  is found (reference 23, Table 73, p. 373) to be 5.0137 whereas the combined mass of an  $\alpha$ -particle plus a neutron would be only  $4.003\ 86 + 1.008\ 93 = 5.012\ 8$ . Thus  $\text{He}^5$  is unstable by 0.9 mMU (milli-mass-units) which is far outside the experimental error (about 0.1–0.2 mMU). It might be argued that the  $\alpha$ -particle group observed in reaction (15) might correspond to an excited state of  $\text{He}^5$ . However, this is extremely improbable because a nucleus of such a simple structure as  $\text{He}^5$  ( $\alpha$ -particle plus neutron) should not have any low-lying excited levels.<sup>24</sup> (This holds both in the  $\alpha$ -particle and the Hartree model of nuclear structure.) Moreover, it would be difficult to explain why the  $\alpha$ -particle group corresponding to the ground state of  $\text{He}^5$  should not have been observed.

The conclusion that the mass of 5.0137 found by W. S. and H. really corresponds to the ground state of  $\text{He}^5$  is supported by considerations of mass defects. In fact, the instability of  $\text{He}^5$  was

<sup>21</sup> H. A. Bethe, Phys. Rev. 54, 436, 955 (1938).

<sup>22</sup> J. H. Williams, W. G. Shepherd and R. O. Haxby, Phys. Rev. 51, 888 (1937).

<sup>23</sup> M. S. Livingston and H. A. Bethe, Rev. Mod. Phys. 9, 247 (1937).

<sup>24</sup> With the possible exception of a doublet structure of the ground state, similar to  $\text{Li}^7$ . However, the doublet separation should probably be much smaller than in  $\text{Li}^7$  because of the loose binding of  $\text{He}^5$ , and presumably both components of the doublet are already contained in the rather broad  $\alpha$ -particle group observed by Williams, Shepherd and Haxby.

first predicted by Atkinson<sup>25</sup> on the basis of such considerations. Considering analogous nuclei, consisting of  $\alpha$ -particles plus one neutron, we find that the last neutron is bound with a binding energy of 5.3 mMU in  $\text{C}^{13}$  and with only 1.8 mMU in  $\text{Be}^9$ . A binding energy of –0.9 mMU in  $\text{He}^5$  fits very well into this series while a positive binding energy would not.

If  $\text{He}^5$  is unstable, this is *a fortiori* true of  $\text{Li}^5$  since the binding energies of these two nuclei should differ by just the Coulomb repulsion between proton and alpha in  $\text{Li}^5$ . This repulsion will be about 0.6–1 mMU, so that  $\text{Li}^5$  is unstable by 1.4–1.8 mMU.

Thus all the nuclear evidence<sup>25a</sup> points to the nonexistence of both  $\text{He}^5$  and  $\text{Li}^5$ . Even if there were no such evidence, astrophysical data themselves would force us to this conclusion, because at a temperature of  $2 \cdot 10^7$  degrees (central temperature of sun) the energy production from the combination of  $\text{He}^4$  and  $\text{H}$  forming  $\text{Li}^5$  would be of the order of  $10^{10}$  ergs/g sec. (cf. §4), as against an observed energy production of 2 ergs/g sec. Only the nonexistence of  $\text{Li}^5$  prevents this enormous production of energy.

### $\text{Be}^6$

This nucleus is certainly unstable, as can be shown by comparing it with the known nucleus  $\text{He}^6$  from which it differs by the interchange of protons and neutrons. The Coulomb energy which is the only difference between the binding energies of the two nuclei can be calculated rather accurately.<sup>21</sup> The instability against disintegration into  $\text{He}^4 + 2\text{H}$  is between 1 and 2.6 mMU.

### $\text{Be}^7$

This nucleus has been observed by Roberts, Heydenburg and Locher.<sup>26</sup> It decays with a

<sup>25</sup> R. d'E. Atkinson, Phys. Rev. 48, 382 (1935).

<sup>25a</sup> Note added in proof:—Recently, F. Joliot and I. Zlotowski (J. de phys. et rad. 9, 403 (1938)) reported the formation of stable  $\text{He}^5$  from the reaction  $\text{He}^4 + \text{H}^2 = \text{He}^5 + \text{H}^1$ . The evidence is based upon the emission of singly charged particles of long range when heavy paraffin is bombarded by  $\alpha$ -particles. However, the number of such particles observed was exceedingly small (only 6 out of a total of 126 tracks). Furthermore, the mass given for  $\text{He}^5$  by Joliot and Zlotowski (5.0106) is irreconcilable with the stability (against neutron emission) of the well-known nucleus  $\text{He}^5$ .

<sup>26</sup> R. B. Roberts, N. P. Heydenburg and G. L. Locher, Phys. Rev. 53, 1016 (1938).

TABLE IV. Corrected and additional nuclear masses, and binding energies.

NUCLEUS	MASS	BINDING ENERGY (mMU)	REFERENCE
$n^1$	1.008 93		19
$He^3$	3.016 99	5.87	18
$H^4$	4.025 4	0.6 $\pm$ 1	
$He^4$	4.003 86		29
$Li^4$	4.026 9	-1 $\pm$ 1	
$He^5$	5.013 7	-0.9 $\pm$ 0.2	23
$Li^6$	5.013 6	-1.6 $\pm$ 0.3	
$Be^6$	6.021 9	-1.8 $\pm$ 0.8	21
$Be^7$	7.019 28	5.7	26
$Be^8$	8.007 80	-0.08 $\pm$ 0.04	28
$B^8$	8.027 4	0.0 $\pm$ 0.4	21
$B^9$	9.016 4	-0.5 $\pm$ 0.2	21
$C^{10}$	10.020 2	3.8	21
$N^{12}$	12.022 5 -24 3	0.0 $\pm$ 0.9	21
$N^{13}$	13.010 08	2.03	19
$O^{14}$	14.013 1	5.1	21

half-life of 43 days (mean life 60 days) and probably only captures  $K$  electrons. Calculations of the Coulomb energy,<sup>21</sup> on the other hand, would make positron emission just possible (positron energy  $\sim 0.1$  mMU). As a compromise, we assume that the mass of  $Be^7$  is just equal to  $Li^7$  plus two electrons, i.e., 7.019 28.

### $Be^8$

The instability of  $Be^8$  against disintegration into two  $\alpha$ -particles has been definitely established by Paneth and Glückauf<sup>27</sup> who have shown that the  $Be^8$  formed in the photoelectric disintegration of  $Be^9$  disintegrates into 2  $He^4$ . Kirchner and Neuert<sup>28</sup> have confirmed this conclusion by investigating the products of the disintegration  $Be^{11} + H = Be^8 + He^4$ . They found that frequently two  $\alpha$ -particles enter the detecting apparatus simultaneously, with a small angle (less than 50°) between their respective directions of flight; this is just what should be expected if the  $Be^8$  formed breaks up into two  $\alpha$ -particles on its way to the detector. From the average angle between the two alphas, the disintegration energy of  $Be^8$  (difference  $Be^8 - 2He^4$ ) was estimated as between 40 and 120 kev.<sup>28a</sup>

<sup>27</sup> F. A. Paneth and E. Glückauf, Nature 139, 712 (1937).

<sup>28</sup> F. Kirchner and H. Neuert, Naturwiss. 25, 48 (1937).

<sup>28a</sup> Note added in proof.—These conclusions are compatible with the new measurements of S. K. Allison, E. R. Graves, L. S. Skaggs and N. M. Smith, Jr. (Phys. Rev. 55, 107 (1939)) on the reaction energy of  $Be^9 + H = Be^8 + H^2$ .

<sup>29</sup> K. T. Bainbridge, Phys. Rev. 53, 922(A) (1938).

### $B^8$

The existence is doubtful; calculation<sup>21</sup> by comparison with its isobar  $Li^8$  gives a binding energy between -0.4 and +0.4 mMU. This nucleus is not very important for astrophysics.

### $B^9$

$B^9$  is almost certainly unstable, as can be shown by calculating<sup>21</sup> the difference in binding energy (Coulomb energy) between it and its isobar  $Be^9$ . The theoretical instability is between 0.3 and 0.7 mMU, 0.3 being almost certainly a lower limit. However, in view of the smallness of this instability, we shall at least discuss what would happen if  $B^9$  were stable (§6). It will turn out that this would make almost no difference at "ordinary" temperatures ( $2 \cdot 10^7$  degrees) and not much even at higher ones ( $10^8$  degrees). For these calculations, we shall assume  $B^9$  to be stable with 0.2 mMU which seems generous.

### $C^{10}$

$C^{10}$  is stable with 4 mMU against  $Be^8 + 2H$ .

### $N^{12}$

$N^{12}$  is doubtful, mainly because the binding energy of its isobar,  $B^{12}$ , is known only very inaccurately (between 2 and 3.3 mMU). Assuming 2 mMU,  $N^{12}$  would probably be unstable, with 3.3 stable.

Table IV summarizes the binding energies of doubtful nuclei, and also gives some nuclear masses supplementary to and correcting those given in reference 23, p. 373.

## §4. REACTION RATES AT $2 \cdot 10^7$ DEGREES

We are now prepared to actually calculate the rate of nuclear reactions under the conditions prevailing in stars. We choose a temperature of twenty million degrees, close to the temperature at the center of the sun. In order to have a figure independent of density and chemical composition, we calculate (cf. 7)

$$P = (m_2/x_2)p/\rho x_1, \quad (16)$$

$P\rho x_1$  gives the probability (per second) that a given nucleus of kind 2 undergoes a reaction with any nucleus of kind 1. If there are no other reactions destroying or producing nuclei of kind 2,  $1/P\rho x_1$  will be the mean life of nuclei of kind 2 in the star.

TABLE V. Probability of nuclear reactions at  $2 \cdot 10^7$  degrees.\*\*

REACTION	$Q$ (mMU)	$\Gamma$ (EV)	$\tau$	$P$ (SEC. $^{-1}$ )	LIFE, FOR $\rho x_1 = 30$
$H + H = H^2 + e^+$	1.53	Ref. 16	12.5	$8.5 \cdot 10^{-21}$	$1.2 \cdot 10^{11}$ yr.
$H^2 + H = He^3$	5.9	1 E	13.8	$1.3 \cdot 10^{-2}$	2 sec.
$H^2 + H = He^4$	21.3	10 E	14.3	$1.7 \cdot 10^{-1}$	0.2 sec.
$He^4 + H = Li^{4*}$	(0.5)	0.02 D	22.7	$3 \cdot 10^{-7}$	1 day
$He^4 + H = Li^{3*}$	(0.2)	0.005 D	23.2	$6 \cdot 10^{-8}$	6 days
$Li^6 + H = He^4 + He^3$	4.1	$5 \cdot 10^8 X$	31.1	$7 \cdot 10^{-3}$	5 sec.
$Li^7 + H = 2 He^4$	18.6	$4 \cdot 10^4 X$	31.3	$6 \cdot 10^{-4}$	1 min.
$Be^7 + H = B^{8?}$	(0.5)	0.02 D	38.1	$6 \cdot 10^{-13}$	2000 yr.
$Be^8 + H = Li^6 + He^4$	2.4	$10^6 X$	38.1	$4 \cdot 10^{-5}$	15 min.
$B^8 + H = C^{10*}$	3.5	2 D	44.6	$2 \cdot 10^{-12}$	5000 yr.
$B^{10} + H = C^{12}$	9.2	10 D	44.6	$10^{-12}$	1000 yr.
$B^{11} + H = 3 He^4$	9.4	$10^6 E$	44.6	$1.2 \cdot 10^{-7}$	3 days
$C^{11} + H = N^{12}$	(0.4)	0.02 D	50.6	$10^{-17}$	$10^8$ yr.
$C^{12} + H = N^{12}$	2.0	$0.6 X$	50.6	$4 \cdot 10^{-16}$	$2.5 \cdot 10^6$ yr.
$C^{12} + H = N^{14}$	8.2	$30 X$	50.6	$2 \cdot 10^{-14}$	$5 \cdot 10^4$ yr.
$N^{14} + H = O^{15}$	7.8	5 D	56.3	$2 \cdot 10^{-17}$	$5 \cdot 10^7$ yr.
$N^{15} + H = C^{12} + He^4$	5.2	$10^6 E$	56.3	$5 \cdot 10^{-13}$	2000 yr.
$O^{16} + H = F^{17}$	0.5	0.02 D	61.6	$8 \cdot 10^{-22}$	$10^{12}$ yr.
$F^{19} + H = O^{16} + He^4$	8.8	$10^6 E$	66.9	$4 \cdot 10^{-17}$	$3 \cdot 10^7$ yr.
$Ne^{22} + H = Na^{23}$	10.7	10 D	71.7	$5 \cdot 10^{-23}$	$2 \cdot 10^{13}$ yr.
$Mg^{24} + H = Al^{27}$	8.0	10 D	81.3	$10^{-26}$	$10^{17}$ yr.
$Si^{20} + H = P^{21}$	7.0	10 D	90.4	$4 \cdot 10^{-30}$	$3 \cdot 10^{20}$ yr.
$Cl^{37} + H = A^{38}$	12.0	10 D	103.1	$5 \cdot 10^{-26}$	$2 \cdot 10^{25}$ yr.
$H^2 + H^2 = He^2 + n$	3.5	$3 \cdot 10^8 X$	15.7	$10^8$	
$Be^7 + H^2 = B^{8?}$	18.5	$10 D'$	45.9	$2 \cdot 10^{-13}$	
$Be^7 + H^3 = B^8 + n^*$	11.9	$10^6 E$	50.7	$2 \cdot 10^{-10}$	
$Be^7 + He^4 = C^{10}$	16.2	$1 D'$	80.5	$3 \cdot 10^{-28}$	
$H^2 + He^4 = Li^6$	1.7	$4 \cdot 10^{-3} Q$	27.5	$3 \cdot 10^{-10}$	
$He^4 + He^4 = Be^7$	1.6	$0.02 D'$	47.3	$3 \cdot 10^{-17}$	
$He^4 + He^4 = Be^{8*}$	(0.05)	$5 \cdot 10^{-9} Q$	50.0	$10^{-24}$	$3 \cdot 10^7$ yr.
$Li^7 + He^4 = B^{11}$	9.1	$1 D'$	71.0	$2.5 \cdot 10^{-24}$	
$Be^7 + He^4 = C^{11}$	8.0	$1 D'$	86	$3 \cdot 10^{-30}$	
$C^{12} + He^4 = O^{16}$	7.8	$1 Q'$	119	$7 \cdot 10^{-43}$	

\*\* The letters in the column giving the level width mean:  $X$  = experimental value;  $D$  = calculated for dipole radiation, from Eq. (12);  $D'$  = dipole radiation with small specific charge,  $1/4$  to  $1/20$  of Eq. (12);  $Q$  = quadrupole radiation, Eq. (12a); and  $E$  = estimate.

\* These reactions are not believed to occur since their product or one of the reactants is unstable. They are listed merely for the sake of discussion.

Table V gives the results of the calculations, based on Eqs. (7) to (9). In the first column, the nuclear reactions are listed. All reactions which seemed of importance in the interior of stars were considered; in addition, some reactions with heavier elements ( $O^{16}$  to  $Cl^{37}$ ) were included in order to show the manner in which the reaction rate decreases. Moreover, seven reactions were listed in spite of the fact that their products or reactants are believed to be (§3) unstable (starred) or doubtful (question mark); these reactions are included in order to discuss the consequences if they did occur.

The second column gives the energy evolution  $Q$  in the reaction, calculated from the masses (reference 23, Table LXXIII, and this paper, Table IV). In the third column, the width  $\Gamma$  determining the reaction rate (cf. §2) is tabulated. Wherever possible, this was taken from experiments (Tables II and III) or from the "empirical formulae" (12), (12a) for the radia-

tion width. For the radiative combination of two nuclei of equal specific charge ( $H^2 + He^4$ ,  $He^4 + He^4$ ,  $C^{12} + He^4$ ) quadrupole radiation was assumed, otherwise dipole radiation.<sup>20</sup> For almost equal specific charge (e.g.,  $Be^7 + He^4$ ), the dipole formula with an appropriate reduction was used. In some instances, the width was estimated by analogy (e.g.,  $N^{15} + H = C^{12} + He^4$ ) or from approximate theoretical calculations ( $H^2 + H = He^4$ ).<sup>21</sup> The way in which  $\Gamma$  was obtained was indicated by a letter in each instance.

The fourth column contains  $\tau$ , as calculated from (8), the fifth  $P$  from (16). The wide variation of  $P$  is evident, also the smallness of  $P$  for  $\alpha$ -particle reactions.

<sup>20</sup> If the combined initial nuclei and the final nucleus have the same parity (as may be the case, e.g., for  $O^{16} + H = F^{17}$ ), it is still possible to have a dipole transition if only the incident particle has orbital momentum one. This does not materially affect its penetrability if  $R > a$  (cf. (4), (5)) which is true in every case where the parities are expected to be the same.

<sup>21</sup> L. I. Schiff, Phys. Rev. 52, 242 (1937).

E.g., the reaction between  $\text{He}^4$  and a nucleus as light as Be is as improbable as between a proton and Si. This arises, of course, from the greater charge and mass of the  $\alpha$ -particle both of which factors reduce its penetrability. The reaction  $\text{He}^4 + \text{He}^4 = \text{Be}^8$  has an exceedingly small probability because of the small frequency and the quadrupole character of the emitted  $\gamma$ -rays. Thus this reaction would not be important even if  $\text{Be}^8$  were stable. On the other hand, the reaction  $\text{He}^4 + \text{H} = \text{Li}^5$  would be extremely probable if  $\text{Li}^5$  existed. The helium in the sun would be "burnt up" completely in about six days, even if rather unfavorable assumptions are made about the probability of the reaction. Similarly, if the energy evolution per process is 0.2 mMU =  $3 \cdot 10^{-7}$  ergs, the energy produced per gram of the star would be

$$(6 \cdot 10^{23}/4) \rho x_{\text{H}} x_{\text{He}} \cdot 3 \cdot 10^{-7} \cdot 6 \cdot 10^{-8}.$$

With  $\rho = 80$ ,  $x_{\text{H}} = 0.35$  and  $x_{\text{He}} = 0.1$ , this would give about  $10^{10}$  ergs/g sec. as against 2 ergs/g sec. observed. This is a very strong additional argument against the existence of  $\text{Li}^5$ .

In the last column of Table V, the mean life is calculated for the various nuclei reacting with protons, by assuming a density  $\rho = 80$  and hydrogen content  $x_1 = 35$  percent, which correspond to the values at the center of the sun.<sup>1</sup> It is seen that, with the exception of H, the lifetimes of all nuclei up to boron are quite short, ranging from a fraction of a second for  $\text{H}^3$  to 1000 years for  $\text{B}^{10}$ . (The life of  $\text{B}^{10}$  may actually be slightly shorter because of the reaction  $\text{B}^{10} + \text{H} = \text{Be}^7 + \text{He}^4$ . See §6.) Of the two lives longer than 1000 years listed, one refers to  $\text{B}^9$  which probably does not exist (§3), the other to  $\text{Be}^7$  which decays by positron emission with a half-life of 43 days.<sup>26</sup> We must conclude that *all the nuclei between H and C, notably  $\text{H}^2$ ,  $\text{H}^3$ ,  $\text{Li}^6$ ,  $\text{Li}^7$ ,  $\text{Be}^9$ ,  $\text{B}^{10}$ ,  $\text{B}^{11}$ , can exist in the interior of stars only to the extent to which they are continuously re-formed by nuclear reactions.* This conclusion does not apply to  $\text{He}^4$  because  $\text{Li}^6$  does not exist. To  $\text{He}^3$  it probably applies whether  $\text{Li}^4$  exists or not, because  $\text{He}^3$  will also be destroyed by combination with  $\text{He}^4$  into  $\text{Be}^7$ , although with a considerably longer period ( $3 \cdot 10^7$  years instead of the 1 day for the reaction giving  $\text{Li}^4$ ).

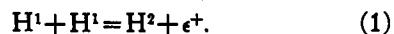
The actual lifetime of carbon and nitrogen is much longer than it would appear from the table because these nuclei are reproduced by the nuclear reactions themselves (§7). This makes their actual lifetime of the order of  $10^{12}$  (or even  $10^{20}$ , cf. §7) years, i.e., long compared with the age of the universe ( $\sim 2 \cdot 10^9$  years). Protons, and all nuclei heavier than nitrogen, also have lives long compared with astronomical times.

### §5. THE REACTIONS FOLLOWING PROTON COMBINATION

In the last section, it has been shown that all elements lighter than carbon, with the exception of H<sup>1</sup> and He<sup>4</sup>, have an exceedingly short life in the interior of stars. Such elements can therefore only be present to the extent to which they are continuously produced in nuclear reactions from elements of longer life. This is in accord with the small abundance of all these elements both in stars and on earth.

Of the two more stable nuclei, He<sup>4</sup> is too inert to play an important rôle. It combines neither with a proton nor with another  $\alpha$ -particle since the product would in both cases be an unstable nucleus. The only way in which He<sup>4</sup> can react at all, is by triple collisions. These will be discussed in the next section and will be shown to be very rare, as is to be expected.

As the only primary reaction between elements lighter than carbon, there remains therefore the reaction between two protons,



According to Critchfield and Bethe,<sup>16</sup> this process gives an energy evolution of 2.2 ergs/g sec. under "standard stellar conditions" (2 · 10<sup>7</sup> degrees,  $\rho = 80$ , hydrogen content 35 percent). The reaction rate under these conditions is (cf. Table V)  $2.5 \cdot 10^{-19}$  sec.<sup>-1</sup>, corresponding to a mean life of  $1.2 \cdot 10^{11}$  years for the hydrogen in the sun. This lifetime is about 70 times the age of the universe as obtained from the red shift of nebulae.

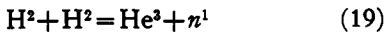
According to the foregoing, any building up of elements out of hydrogen will have to start with reaction (1). The deuteron will capture another proton,



This reaction follows almost instantaneously upon (1), with a delay of only 2 sec. (Table V). There is, therefore, always statistical equilibrium between protons and deuterons, the concentrations (by number of atoms) being in the ratio of the respective lifetimes. This makes the concentration of deuterons (by weight) equal to

$$x(H^2) = x(H^1) \cdot \frac{2 \cdot 8.5 \cdot 10^{-21}}{1.3 \cdot 10^{-2}} = 1.3 \cdot 10^{-18} x(H^1) \quad (18)$$

(cf. Table V). The relative probability of the reaction



as compared with (17), is then

$$p_n = \frac{1}{4} \frac{P(H^2 + H^2 = He^3 + n^1)}{P(H^2 + H = He^3)} \cdot \frac{x(H^2)}{x(H^1)} = \frac{10^3 \cdot 1.3 \cdot 10^{-18}}{4 \cdot 1.3 \cdot 10^{-2}} = 2 \cdot 10^{-14}. \quad (19a)$$

(One factor  $\frac{1}{2}$  comes from the fact that in (19) two nuclei of the same kind interact; another is the atomic weight of  $H^2$ .) Thus one neutron is produced for about  $5 \cdot 10^{13}$  proton combinations.

The further development of the  $He^3$  produced according to (17) depends on the question of the stability of  $Li^4$  and of the relative stability of  $H^3$  and  $He^3$ .

#### Assumption A: $Li^4$ stable

In this case, the  $He^3$  will capture another proton, *viz.*:



With the assumptions made in Table V, the mean life of  $He^3$  would be 1 day. The  $Li^4$  would then emit a positron:



With an assumed stability of  $Li^4$  of 0.5 mMU compared with  $He^3 + H^1$ , the maximum energy of the positrons in (20a) would be  $20.8$  mMU =  $19.4$  Mev (including rest mass) which would be by far the highest  $\beta$ -ray energy known. The lifetime of  $Li^4$  may accordingly be expected to be a small fraction of a second (half-life =  $1/500$  sec. for an allowed transition in the Fermi theory).

The most important consequence of the stability of  $Li^4$  would be that only a fraction of the mass difference between four protons and an  $\alpha$ -particle would appear as usable energy. For in the  $\beta$ -emission (20a) the larger part of the energy is, on the average, given to the neutrino which will in general leave the star without giving up any of its energy

(see below). According to the Konopinski-Uhlenbeck theory, which is in good agreement with the observed energy distribution in  $\beta$ -spectra, the neutrino receives on the average  $5/8$  of the total available energy if the latter is large. In our case, this would be  $13.0$  mMU. Adding  $0.2$  mMU for the neutrino emitted in process (1), we find that altogether  $13.2$  mMU energy is lost to neutrinos, of a total of  $28.7$  mMU developed in the formation of an  $\alpha$ -particle out of four protons and two electrons. Thus the observable energy evolution is only  $15.5$  mMU, i.e.,  $54$  percent of the total. Therefore, if  $Li^4$  is stable, process (1) would give only  $1.2$  ergs/g sec. instead of  $2.2$  (under "standard" conditions).<sup>16</sup>

The neutrinos emitted will have some chance of producing neutrons in the outer layers of the star. It seems reasonable to assume that a neutrino has no other interaction with matter than that implied in the  $\beta$ -theory. Then a free neutrino ( $\nu$ ) will cause only "reverse  $\beta$ -processes"<sup>17</sup> of which the simplest and most probable is



This process is endoergic with  $1.9$  mMU and is therefore caused only by fast neutrinos such as those from  $Li^4$ . The cross section is according to the Fermi theory

$$\sigma = \pi^2 (\hbar/mc)^3 \cdot 0.9 \cdot 10^{-4} c^{-1} W(W^2 - 1)^{\frac{1}{2}} = 1.7 \cdot 10^{-48} W(W^2 - 1)^{\frac{1}{2}} \text{ cm}^2, \quad (22)$$

where  $W$  is the energy of the emitted positron, including rest mass, in units of  $mc^2$ . In reaction (21), this is the neutrino energy minus  $1.35$  mMU. For the  $Li^4$  neutrinos, the average cross section comes out to be

$$\sigma_{Av} = 2.5 \cdot 10^{-43} \text{ cm}^2 \quad (22a)$$

per proton, and the probability of process (21) for a neutrino starting from the center of the star

$$p = 6 \cdot 10^{23} \cdot \sigma_{Av} x_H \int_0^R \rho dr = 1.5 \cdot 10^{-19} x_H \int_0^R \rho dr, \quad (22b)$$

where  $\rho(r)$  is the density (in g/cm<sup>3</sup>) at the distance  $r$  from the center of the star. For the sun,  $p = 1.6 \cdot 10^{-7}$ . This means that  $1.6 \cdot 10^{-7}$  of the neutrinos emitted will cause reaction (21) before leaving the sun, and that the number of neutrons formed is  $1.6 \cdot 10^{-7}$  times the number of proton combinations (1).

A further consequence of (20, 20a) would be that ordinarily no nuclei heavier than 4 mass units are formed at all, even as intermediate products. Such nuclei would only be produced in the rare cases when  $H^2$  or  $He^3$  capture an  $\alpha$ -particle rather than a proton, according to the reactions



and



Under the favorable assumption that the concentration of  $He^4$  is the same as of  $H^1$  (by weight), the fraction of  $H^2$  forming  $Li^6$  is (cf. Table V)

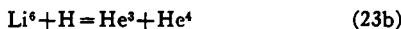
$$p(Li^6) = 3 \cdot 10^{-10} / 1.3 \cdot 10^{-2} = 2 \cdot 10^{-8} \quad (23a)$$

the fraction of  $He^3$  giving  $Be^7$  is

$$p(Be^7) = 3 \cdot 10^{-17} / 3 \cdot 10^{-7} = 10^{-10}. \quad (24a)$$

<sup>16</sup> H. A. Bethe and R. Peierls, Nature 133, 689 (1934).

Most of the  $\text{Li}^6$  will give rise to the well-known reaction



and most of the  $\text{Be}^7$  will go over into  $\text{Li}^7$  which in turn reacts with a proton to give two  $\alpha$ -particles. Only occasionally,  $\text{Li}^6$ ,  $\text{Be}^7$  or  $\text{Li}^7$  will capture an  $\alpha$ -particle and thus form heavier nuclei. It can be shown (cf. assumption B) that  $\text{Li}^7$  is the most efficient nucleus in this respect. Therefore, the amount of heavier elements formed is determined by  $\text{Be}^7$ , the mother substance of  $\text{Li}^7$ , and is thus  $10^{-10}$  times the amount formed with assumption B.

#### Assumption B: $\text{Li}^6$ unstable, $\text{He}^3$ more stable than $\text{H}^3$

This assumption seems to be the most likely according to available evidence. The *only* reaction which the  $\text{He}^3$  can undergo, is then (24), i.e., each proton combination leads to the formation of a  $\text{Be}^7$  nucleus. The most probable mode of decay of this nucleus is by electron capture, leading to  $\text{Li}^7$ . The lifetime of  $\text{Be}^7$  (half-life) is 43 days<sup>26</sup> in the complete atom, and 10 months at the center of the sun (cf. 14, 14a). This makes the mean life = 14 months and the reaction rate  $2.8 \cdot 10^{-8} \text{ sec.}^{-1}$ . The capture of a proton by  $\text{Be}^7$  would, even if the product  $\text{B}^8$  is stable, be 2000 times slower (Table V). Each electron capture by  $\text{Be}^7$  is accompanied by the emission of a neutrino of energy  $\sim 2mc^2 = 1.1 \text{ mMU}$  (when  $\text{Li}^7$  is left in its excited state, which happens rather rarely, the neutrino receives only 0.6 mMU). The total energy lost to neutrinos (including process 1) will therefore be very small in this case ( $\sim 1.3 \text{ mMU per } \alpha\text{-particle formed}$ , i.e.,  $4\frac{1}{2}$  percent of the total energy evolution) and practically the full mass energy will be transformed into heat radiation. The  $\text{Li}^7$  formed by electron capture of  $\text{Be}^7$  will cause the well-known reaction



and have (Table V) a mean life of only 1 minute at  $2 \cdot 10^7$  degrees.

The reaction chain described leads, as in the case of assumption A, to the building up of one  $\alpha$ -particle out of four protons and two electrons, for each process (1). No nuclei heavier than  $\text{He}^4$  are formed permanently. Such nuclei can be produced only by branch reactions alternative to the main chain described. These will be discussed in the following.

*a. Reactions with protons.*—When  $\text{Li}^7$  reacts with slow protons, the result is not always two  $\alpha$ -particles, but, in one case out of about<sup>27</sup> 5000, radiative capture, giving  $\text{Be}^8$ . However,  $\text{Be}^8$  will disintegrate again into two  $\alpha$ -particles (§3), and during its life of about  $10^{-12} \text{ sec.}$ , the probability of its reacting with another particle (e.g., capture of another proton) is exceedingly small ( $\sim 10^{-24}$ ). Similarly,  $\text{Be}^7$  will, in one out of about 2000 cases (see above) capture a proton and form  $\text{B}^8$  if that nucleus exists. However,  $\text{B}^8$

<sup>26</sup> It was assumed that radiative capture takes place only through the resonance level at 440 kv proton energy. The proton width of this level was taken as 11 kv, the radiation width as 40 ev.

will again go over into  $\text{Be}^8$ , by positron emission, and two alphas will again be the final result.

At this place, obviously, stability of  $\text{Be}^8$  would increase the yield of heavy nuclei. Then one stable  $\text{Be}^8$  would be formed for 5000 proton combinations; and, if  $\text{B}^8$  is also assumed to be stable, every  $\text{Be}^8$  goes over into  $\text{B}^9$ . Since about one out of  $3 \cdot 10^8 \text{ B}^9$  gives a  $\text{C}^{12}$  (§6), the number of heavy nuclei ( $\text{C}^{12}$ ) formed would be  $\sim 10^{-12}$  per  $\alpha$ -particle. This would be the highest yield obtainable. However,  $\text{Be}^8$  is known to be unstable (§3).

*b. Reactions with  $\alpha$ -particles.*—The only abundant light nucleus other than the proton is  $\text{He}^4$ . The only reaction possible between an  $\alpha$ -particle and  $\text{Li}^7$  or  $\text{Be}^7$  is radiative capture, *viz.*



The probability of formation of  $\text{B}^{11}$  and  $\text{C}^{11}$  is (Table V)

$$p(\text{B}^{11}) = \frac{P(\text{Li}^7 + \text{He}^4)}{P(\text{Li}^7 + \text{H})} = \frac{2.5 \cdot 10^{-24}}{6 \cdot 10^{-4}} = 4 \cdot 10^{-21}, \quad (26b)$$

$$p(\text{C}^{11}) = \frac{P(\text{Be}^7 + \text{He}^4)}{P(\text{Be}^7 + \epsilon = \text{Li}^7)} = \frac{14 \text{ months}}{3 \cdot 10^{20} \text{ yr.}} = 4 \cdot 10^{-21}. \quad (26c)$$

Thus the formation of  $\text{B}^{11}$  is about as probable as that of  $\text{C}^{11}$ ; the effect of the lower potential barrier of  $\text{Li}^7$  for  $\alpha$ -particles is compensated by its shorter life. The  $\text{C}^{11}$  will, of course, also give  $\text{B}^{11}$  by positron emission.

The  $\text{B}^{11}$  will react with protons in two ways, *viz.*



The branching ratio is about  $10^4 : 1$  in favor of (27) (calculated from experimental data). Thus there will be one  $\text{C}^{12}$  nucleus formed for about  $10^{24}$   $\alpha$ -particles. The building up of heavier nuclei, even in this most favorable case, is therefore exceedingly improbable.

*c. Reactions with  $\text{He}^4$ .*—Since  $\text{He}^4$  has a rather long life  $3 \cdot 10^7$  years, Table V) and penetrates more easily through the potential barrier than the heavier  $\text{He}^4$ , it may be considered as an alternative possibility. However, the probability of formation of  $\text{C}^{10}$  from  $\text{Be}^7 + \text{He}^4$  is only 100 times greater than that of  $\text{C}^{11}$  from  $\text{Be}^7 + \text{He}^4$  (Table V) if the concentrations of  $\text{He}^4$  and  $\text{He}^4$  are equal. Actually, that of  $\text{He}^4$  is only about  $3 \cdot 10^{-4}$  (life of  $\text{He}^4$  divided by life of protons) so that this process is  $1/30$  as probable as (26a). For  $\text{Li}^7 + \text{He}^4$ , the situation is even less favorable.

*d. Reactions with  $\text{H}^2$ .*—Deuteron capture by  $\text{Be}^7$  would lead to  $\text{B}^9$  whose existence is very doubtful. The probability per second would be (cf. Table V and Eq. (18))

$$2 \cdot 10^{-12} p_x(\text{H}^2) = 2 \cdot 10^{-12} \cdot 30 \cdot 1.3 \cdot 10^{-18} = 10^{-29}, \quad (28)$$

which is only  $1/10$  of the probability of (26a) (Table V). Moreover, most of the  $\text{B}^9$  formed reverts to  $\text{He}^4$  (§6) so that the contribution of this process is negligible.

*e. Reactions with  $\text{He}^4$  in situ nascendi.*—The process (25) produces continuously fast  $\alpha$ -particles which need not penetrate through potential barriers. These  $\alpha$ -particles have a range of 8 cm each in standard air, corresponding to 16 cm =  $0.02 \text{ g/cm}^2$  for both. In stars, with their large hydrogen content, a somewhat smaller figure must be used

since hydrogen has a greater stopping power per gram; we take  $0.01 \text{ g/cm}^2$ . The cross section for fast particles is about

$$\sigma = \pi R^2 \frac{\Gamma}{\hbar^2 / MR^2}. \quad (29)$$

With  $\Gamma = 1 \text{ volt}$  (Table V) and  $R = 3.6 \cdot 10^{-13} \text{ cm}$  (Eq. (10)), this gives  $\sigma = 1.3 \cdot 10^{-31} \text{ cm}^2$ . The number of  $\text{Be}^7$  atoms per gram is

$$6 \cdot 10^{33} x(\text{Be}^7) = 6 \cdot 10^{33} \cdot \frac{14 \text{ months}}{1.2 \cdot 10^{11} \text{ yr}} x(\text{H}) = 2 \cdot 10^{12} \quad (29a)$$

with  $x(\text{H}) = 0.35$ . This gives for the number of processes (26a) per proton combination:

$$0.01 \cdot 2 \cdot 10^{12} \cdot 1.3 \cdot 10^{-31} = 2.5 \cdot 10^{-21}, \quad (29b)$$

which is about the same as the formation of  $\text{C}^{11}$  or  $\text{B}^{11}$  by capture of slow alphas (cf. 26b, c).

Returning to the main reaction chain in the case of our assumption B, we note that the formation of  $\text{Be}^7$  (Eq. (24)) is a very slow reaction, requiring  $3 \cdot 10^7$  years at "standard" conditions ( $2 \cdot 10^6$  degrees). At lower temperatures, the reaction will be still slower and, finally, it will take longer than the past life of the universe ( $\sim 2 \cdot 10^9$  years). In this case, the amount of  $\text{He}^3$  present will be much smaller than its equilibrium value (provided there was no  $\text{He}^3$  "in the beginning") and the energy production due to reactions (24), (25) will be reduced accordingly. Ultimately, at very low temperatures ( $< 12 \cdot 10^6$  degrees), the reaction  $\text{H} + \text{H}$  will lead only to  $\text{He}^3$ , and will therefore give an energy production of only  $7.2 \text{ mMU}$ , i.e., only one-quarter of the high temperature value,  $27.4 \text{ mMU}$ .

#### Assumption C: $\text{H}^3$ more stable than $\text{He}^3$

In this case,  $\text{He}^3$  will be able to capture an electron,

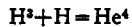


Under the assumption that a difference in mass of 0.1 electron mass exists between  $\text{He}^3$  and  $\text{H}^3$ , the probability of (30) is, according to (14a),

$$\rho(\text{H}^3) = 1.5 \cdot 10^{-11} \text{ sec.}^{-1} \quad (30a)$$

for a density  $\rho = 80$  and 35 percent hydrogen content. This corresponds to a mean life of  $\sim 2000$  years. The electron capture is therefore about  $10^4$  times more probable than the formation of  $\text{Be}^7$  according to (24). This ratio will be reversed at temperatures  $> 4 \cdot 10^7$  since (30) is independent of  $T$  and the probability of (24) increases as  $T^3$ .

$\text{H}^3$  will capture a proton and form  $\text{He}^4$ ,



with a mean life of about 0.2 seconds. This way of formation of  $\text{He}^4$  from reaction (1) is probably the most direct of all. As in B, practically no energy is lost to neutrinos.

The formation of heavier elements goes as in B, but now there is only one  $\text{Be}^7$  formed for  $10^4$  proton combination processes. This reduces the probability of formation of  $\text{C}^{12}$  by another factor  $10^4$ , to one  $\text{C}^{12}$  in  $10^{28}$  alphas.

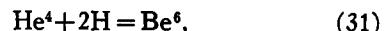
The  $\text{H}^3$  itself does not contribute appreciably to the building up of elements. It is true that the reaction  $\text{Be}^7 + \text{H}^3 = \text{B}^9 + n^1$  is about 100 times as probable as  $\text{Be}^7 + \text{H}^2 = \text{B}^9$

(considering the shorter life of  $\text{H}^3$ ), and therefore 10 times as probable as (26a). However, most of the  $\text{B}^9$  reverts to  $\text{He}^4$  (cf. §6) so that (26) and (26a) remain the most efficient processes for building up  $\text{C}^{12}$ .

Summarizing, we find that the formation of nuclei heavier than  $\text{He}^4$  can occur only in negligible amounts. One  $\text{C}^{12}$  in  $10^{24}$   $\alpha$ -particles and one neutron in  $10^{14}$   $\alpha$ -particles are the yields when  $\text{Li}^4$  is unstable, one  $\text{C}^{12}$  in  $10^{34}$  alphas and one neutron in  $10^7$  alphas when  $\text{Li}^4$  is stable. The reason for the small probability of formation of  $\text{C}^{12}$  is twofold: First, any nonradioactive nucleus between He and C, i.e.,  $\text{Li}^{6,7}$ ,  $\text{Be}^9$ ,  $\text{B}^{10,11}$ , reacting with protons will give  $\alpha$ -particle emission rather than radiative capture so that a disintegration takes place rather than a building up. This will no longer be the case for heavier nuclei so that for these a building up is actually possible. Second, the instability of  $\text{Be}^8$  causes a gap in the list of stable nuclei which is the harder to bridge because  $\text{Be}^8$  is very easily formed in nuclear reactions (small mass excess). On the other hand, the instability of  $\text{He}^5$  and  $\text{Li}^5$  is of no influence because  $\text{Be}^7$  and  $\text{Li}^7$  are stages in the ordinary chain of nuclear reactions.

#### §6. TRIPLE COLLISIONS OF ALPHA-PARTICLES

In the preceding section, we have shown that collisions with protons alone lead practically always to the formation of  $\alpha$ -particles. In order that heavier nuclei be formed, use must therefore certainly be made of the  $\alpha$ -particles themselves. However, collisions of an  $\alpha$ -particle with one other particle, proton or alpha, do not lead to stable nuclei. Therefore we must assume triple collisions, of which three types are conceivable:



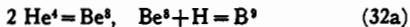
The first of these reactions leads to a nucleus which is certainly unstable ( $\text{Be}^6$ ). Even if it were stable, it would not offer any advantages over  $\text{Be}^7$  which is formed as a consequence of the proton combination (1). The second reaction leads to  $\text{B}^9$  which is probably also unstable. However, since this is not absolutely certain, we

\* G. Breit and E. Wigner, Phys. Rev. 49, 519 (1936).

shall discuss this process in the following. The last process leads directly to  $C^{12}$ , but since it involves a rather large potential barrier for the last  $\alpha$ -particle, it is very improbable at  $2 \cdot 10^7$  degrees (see below).

### The formation of $B^9$

The probability of this process is enhanced by the well-known resonance level of  $Be^8$ , which corresponds to a kinetic energy of about  $E = 50$  kev of two  $\alpha$ -particles. The formation of  $B^9$  occurs in two stages,



with a time interval of about  $10^{-13}$  sec. (life of  $Be^8$ ). The process can be treated with the usual formalism for resonance disintegrations, the compound nucleus being  $Be^8$ . This nucleus can "disintegrate" in two ways, (a) into two  $\alpha$ -particles, (b) with proton capture. We denote the respective widths of the  $Be^8$  level by  $\Gamma_\alpha$  and  $\Gamma_H$ ; the latter is given by the ordinary theory of thermonuclear processes, i.e.,

$$\Gamma_H = \hbar p m_H / x_H, \quad (34)$$

where  $p$  is given by (4), and the subscripts 1 and 2 denote  $H^1$  and  $Be^8$ , respectively.

The cross section of the resonance disintegration becomes then

$$\sigma = \pi \lambda^2 \frac{\Gamma_\alpha \Gamma_H}{(E - E_r)^2 + \frac{1}{4}(\Gamma_\alpha + \Gamma_H)^2}. \quad (35)$$

$E_r$  is the resonance energy.  $\Gamma_\alpha$  is much larger than  $\Gamma_H$  (corresponding to about  $10^{13}$  and  $10^{-11}$  sec. $^{-1}$ , respectively) but very small compared with  $E_r$  (about  $10^{-2}$  against  $5 \cdot 10^4$  volts). The resonance is thus very sharp, and, integrating over the energy, we obtain for the total number of processes per cm $^3$  per sec. simply

$$\rho \dot{\rho} = B(E_r) v_r \pi \lambda^2 2 \pi \Gamma_H. \quad (36)$$

Here  $B(E)dE$  is the number of pairs of  $\alpha$ -particles with relative kinetic energy between  $E$  and  $E+dE$  per cm $^3$ , viz.

$$B(E) = \frac{1}{2} \left( \frac{\rho x_\alpha}{m_\alpha} \right)^2 \frac{2}{\pi^2} \frac{E^2}{(kT)^2} e^{-E/kT} \quad (36a)$$

( $x_\alpha$  = concentration of  $He^4$  by weight). Combining (36), (36a) and (34), (4), we find

$$\rho(B^9) = \frac{16\pi^{3/2}}{3^{5/2}} \frac{\rho^2 x_\alpha^2 x_H}{m_\alpha^{1/2} m_H} \frac{\hbar^3 \Gamma_{rad}}{(kT)^{3/2}} a R^2 r^2 \times \exp \{4(2R/a)^2 - \tau - E_r/kT\}, \quad (37)$$

where  $\Gamma_{rad}$  is the radiation width for the process  $Be^8 + H \rightarrow B^9$ . Numerically, (37) gives for the decay constant of hydrogen the value

$$\rho m_H / x_H = 1.00 \cdot 10^{-4} (\rho x_\alpha)^2 \Gamma \varphi T^{-1} e^{-11.7 E_r/T} r^2 e^{-\tau}, \quad (37a)$$

where  $T$  is measured in millions of degrees, the resonance energy  $E_r$  of  $Be^8$  in kilo-electron-volts and  $\Gamma$  in ev. The quantities  $\Gamma$ ,  $\varphi$  and  $\tau$  refer to the process  $Be^8 + H \rightarrow B^9$ . If

there were no resonance level of  $Be^8$ , (37) would be replaced by

$$\rho(B^9) = \frac{8}{243} \frac{\rho^2 x_\alpha^2 x_H}{m_\alpha^2 m_H} \frac{\hbar^3 \Gamma_{rad}}{k} a R^2 a' R' r^2 r'^2 \times \exp \{(32R/a)^2 + (32R'/a')^2 - \tau - \tau'\}, \quad (38)$$

where the primed quantities refer to the reaction  $2 He^4 \rightarrow Be^8$ , the unprimed ones to  $Be^8 + H \rightarrow B^9$ . Numerically, (38) gives

$$\rho m_H / x_H = 2.0 \cdot 10^{-11} (\rho x_\alpha)^2 \Gamma \varphi r^2 e^{-\tau} \varphi' r'^2 e^{-\tau'}. \quad (38a)$$

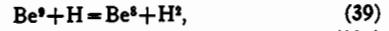
Assuming  $T = 20$ ,  $\rho = 80$ ,  $x_\alpha = 0.25$ ,  $\Gamma = 0.02$  electron-volts, we obtain for the probability of formation of  $B^9$  per proton per second:

$$\begin{aligned} \rho m_H / x_H &= 2 \cdot 10^{-25} \text{ for resonance, } E_r = 25 \text{ kev} \\ &\quad 10^{-21} \text{ for resonance, } E_r = 50 \text{ kev} \\ &\quad 4 \cdot 10^{-28} \text{ for resonance, } E_r = 75 \text{ kev} \\ &\quad 2 \cdot 10^{-44} \text{ for resonance, } E_r = 100 \text{ kev} \\ &\quad 5 \cdot 10^{-62} \text{ for nonresonance.} \end{aligned}$$

The value 25 kev for the resonance level must probably be excluded on the basis of the experiments of Kirchner and Neuert.<sup>28</sup> But even for this low value of the resonance energy, the probability of formation of  $B^9$  is only  $10^{-6}$  times that of the proton combination  $H + H \rightarrow H^2 + e^+$  (Table V,  $\rho x_1 = 30$ ). With  $E_r = 50$  kev which seems a likely value, the ratio becomes  $4 \cdot 10^{-13}$ . On the other hand, the building up of  $B^9$  (if this nucleus exists) would still be the most efficient process for obtaining heavier elements (see below).

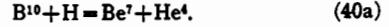
### Reactions of $B^9$

It can easily be seen<sup>21</sup> that  $B^9$  cannot be positron-active but can only capture electrons if it exists at all. If  $B^9$  is stable by 0.3 mMU, the energy evolution in electron capture would be just one electron mass. The decay constant of  $B^9$  (for  $\beta$ -capture) is then, according to (14a),  $1.5 \cdot 10^{-9}$  sec. $^{-1}$  ( $\rho = 80$ ,  $x_H = 0.35$ ) corresponding to a lifetime of about 20 years. On the other hand, the lifetime with respect to proton capture (Table V) is 5000 years. Therefore, ordinarily  $B^9$  will go over into  $Be^8$ . This nucleus, in turn, will in general undergo one of the two well-known reactions:



Only in one out of about  $10^8$  cases,  $B^{10}$  will be formed by radiative proton capture. Therefore the more efficient way for building up heavier elements will be the direct proton capture by  $B^9$ , leading to  $C^{10}$ , which occurs in one out of about 300 cases.

The  $C^{10}$  produced will go over into  $B^{10}$  by positron emission.  $B^{10}$  may react in either of the following ways:



The reaction energy of (40a) is (cf. Table VII, §8) 1.2 mMU; the penetrability of the outgoing alphas about 1/40 (same table), therefore the probability of the particle reaction (40a) will be about 100 times that of the capture reaction (40).

The  $C^{11}$  from (40) will emit another positron. The resulting  $B^{11}$  reacts with protons as follows:



Both reactions are well-known experimentally. Reaction (41) has a resonance at 160 kev. From the width of this resonance and the experimental yields, the probability of (41) with low energy protons is about 1 in 10,000 (i.e., the same as for nonresonance). Altogether, about one  $B^9$  in  $3 \cdot 10^8$  will transform into  $C^{12}$ .

With a resonance energy of  $Be^8$  of 50 kev, and  $2 \cdot 10^7$  degrees, there will thus be about one  $C^{12}$  formed for  $10^{21}$   $\alpha$ -particles if  $B^9$  is stable. This is better than any other process but still negligibly small.

At higher temperatures, the formation of  $B^9$  will become more probable and will, for  $T > 10^8$ , exceed the probability of the proton combination. At these temperatures (actually already for  $T > 3 \cdot 10^7$ ) the  $B^9$  will rather capture a proton (giving  $C^{10}$ ). Even then, there remain the unfavorable branching ratios in reactions (40), (40a) and (41), (41a),<sup>55</sup> so that there will still be only one  $C^{12}$  formed in  $10^6$  alphas. Thus even with  $B^9$  stable and granting the excessively high temperature, the amount of heavy nuclei formed is extremely small.

#### Direct formation of $C^{12}$

$C^{12}$  may be formed directly in a collision between 3  $\alpha$ -particles. The calculation of the probability is exactly the same as for the formation of  $B^9$ . The nonresonance process gives about the same probability as a resonance of  $Be^8$  at 50 kev. With  $\rho = 80$ ,  $x_\alpha = \frac{1}{4}$ ,  $\Gamma = 0.1$  electron-volt,  $T = 2 \cdot 10^7$  degrees, the probability is  $10^{-66}$  per  $\alpha$ -particle, i.e., about  $10^{-37}$  of the proton combination reaction (1). This gives an even smaller yield of  $C^{12}$  than the chains described in this and the preceding section. The process is strongly temperature-dependent, but it requires temperatures of  $\sim 10^9$  degrees to make it as probable as the proton combination (1).

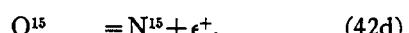
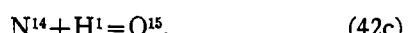
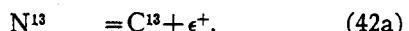
The considerations of the last two sections show that there is no way in which nuclei heavier than helium can be produced permanently in the interior of stars under present conditions. We can therefore drop the discussion of the building up of elements entirely and can confine ourselves to the energy production which is, in fact, the only observable process in stars.

#### §7. THE CARBON-NITROGEN GROUP

In contrast to lighter nuclei,  $C^{12}$  is not permanently destroyed when it reacts with protons;

<sup>55</sup> The reaction  $C^{11} + H = N^{12}$  becomes more probable than  $C^{11} = B^{11} + e^+$  only at  $T > 3 \cdot 10^8$  degrees. The branching ratio in (40), (40a) may perhaps be slightly more favorable because the effect of the potential barrier in (40a) may be stronger.

instead the following chain of reactions occurs



Thus the  $C^{12}$  nucleus is reproduced. The reason is that the alternative reactions producing  $\alpha$ -particles, *viz.*



are all strongly forbidden energetically (Table VII, §8). This in turn is due to the much greater stability of the nuclei in the carbon-nitrogen group as compared with the beryllium-boron group, and is in contrast to the reactions of Li, Be and B with protons which all lead to emission of  $\alpha$ -particles.

The cyclical nature of the chain (42) means that practically no carbon will be consumed. Only in about 1 out of  $10^4$  cases,  $N^{15}$  will capture a proton rather than react according to (42e). In this case,  $O^{16}$  is formed:



However, even then the  $C^{12}$  is not permanently destroyed, because except in about one out of  $5 \cdot 10^7$  cases,  $O^{16}$  will again return to  $C^{12}$  (cf. §8). Thus there is less than one  $C^{12}$  permanently consumed for  $10^{12}$  protons. Since the concentration of carbon and nitrogen, according to the evidence from stellar spectra, is certainly greater than  $10^{-12}$  this concentration does not change noticeably during the evolution of a star. *Carbon and nitrogen are true catalysts; what really takes place is the combination of four protons and two electrons into an  $\alpha$ -particle.*

A given  $C^{12}$  nucleus will, at the center of the sun, capture a proton once in  $2.5 \cdot 10^6$  years (Table V), a given  $N^{14}$  once in  $5 \cdot 10^7$  years. These times are short compared with the age of the sun. Therefore the cycle (42) will have re-

TABLE VI. Central temperatures necessary for giving observed energy production in sun, with various nuclear reactions.

REACTION	T (MILLION DEGREES)
$H^2 + H = He^3$	0.36
$He^4 + H = Li^5$	2.1
$Li^7 + H = 2He^4$	2.2
$Be^9 + H = Li^4 + He^4$	3.3
$B^{10} + H = C^{11}$	9.2
$B^{11} + H = 3He^4$	5.5
$C^{12} + H = N^{13}$	15.5
$N^{14} + H = O^{15}$	18.3
$O^{16} + H = F^{17}$	32
$Ne^{22} + H = Na^{23}$	37

peated itself many times in the history of the sun, so that statistical equilibrium has been established between all the nuclei occurring in the cycle, *viz.*  $C^{12}C^{13}N^{13}N^{14}N^{14}O^{15}$ . In statistical equilibrium, the concentration of each nucleus is proportional to its lifetime. Therefore  $N^{14}$  should have the greatest concentration,  $C^{12}$  less, and  $C^{13}N^{15}$  still less. (The concentration of the radioactive nuclei  $N^{13}$  and  $O^{15}$  is, of course, very small, about  $10^{-12}$  of  $N^{14}$ ). A comparison of the observed abundances of C and N is not very conclusive, because of the very different chemical properties. However, a comparison of the isotopes of each element should be significant.

In this respect, the result for the carbon isotopes is quite satisfactory.  $C^{13}$  captures slow protons about 70 times as easily as  $C^{12}$  (experimental value!), therefore  $C^{12}$  should be 70 times as abundant. The actual abundance ratio is 94 : 1. The same fact can be expressed in a more "experimental" way: In equilibrium, the number of reactions (42) per second should be the same as of (42b). Therefore, if a natural sample of terrestrial carbon (which is presumed to reproduce the solar equilibrium) is bombarded with protons, equally many captures should occur due to each carbon isotope. This is what is actually found experimentally;<sup>13</sup> the equality of the  $\gamma$ -ray intensities from  $C^{12}$  and  $C^{13}$  is, therefore, not accidental.<sup>14</sup>

The greater abundance of  $C^{12}$  is thus due to the smaller probability of proton capture which in turn appears to be due to the smaller  $h\nu$  of

<sup>13</sup> It would be tempting to ascribe similar significance to the equality of intensity of the two  $\alpha$ -groups from natural Li bombarded by protons ( $Li^6 + H = He^4 + He^3$ ,  $Li^7 + H = 2He^4$ ). However, the lithium isotopes do not seem to be genetically related as are those of carbon.

the capture  $\gamma$ -ray. Thus the great energetic stability of  $C^{12}$  actually makes this nucleus abundant. However, it is not because of a Boltzmann factor as has been believed in the past, but rather because of the small energy evolution of the proton capture reaction.

In nitrogen, the situation is different. Here  $N^{14}$  is energetically less stable (has higher mass excess) than  $N^{15}$  but is more abundant in spite of it (abundance ratio  $\sim 500 : 1$ ). This must be due to the fact that  $N^{15}$  can give a  $p - \alpha$  reaction while  $N^{14}$  can only capture a proton; particle reactions are always much more probable than radiative capture. Thus the greater abundance of  $N^{14}$  is due not to its own small mass excess but to the large mass excess of  $C^{11}$  which would be the product of the  $p - \alpha$  reaction (43b).

Quantitative data on the nitrogen reactions (42c), (42e) are not available, the figures in Table V are merely estimates. If our theory about the abundance of the nitrogen isotopes is correct, the ratio of the reaction rates should be 500 : 1, i.e., either  $N^{14} + H = O^{15}$  must be more probable<sup>15a</sup> or  $N^{15} + H = C^{12} + He^4$  less probable than assumed in Table V. Experimental investigations would be desirable.

Turning now to the energy evolution, we notice that the cycle (42) contains two radioactive processes ( $N^{13}$  and  $O^{15}$ ) giving positrons of 1.3<sub>s</sub> and 1.8<sub>s</sub> mMU maximum energy, respectively. If we assume again that  $\frac{1}{2}$  of the energy is, on the average, given to neutrinos, this makes 2.0 mMU neutrino energy per cycle, which is 7 percent of the total energy evolution (28.7 mMU). There are therefore  $4.0 \cdot 10^{-6}$  ergs available from each cycle. (It may be mentioned that the neutrinos emitted have too low energy to cause the transformation of protons into neutrons according to (21).)

The duration of one cycle (42) is equal to the sum of the lifetimes of all nuclei concerned, i.e., practically to the lifetime of  $N^{14}$ . Thus each  $N^{14}$  nucleus will produce  $4.0 \cdot 10^{-6}$  erg every  $5 \cdot 10^7$  years, or  $3 \cdot 10^{-20}$  erg per second. Under the

<sup>15a</sup> Note added in proof.—In this case, the life of  $N^{14}$  in the sun might actually be shorter, and its abundance smaller than that of  $C^{12}$ . Professor Russell pointed out to me that this would be in better agreement with the evidence from stellar spectra. Another consequence would be that a smaller abundance of  $N^{14}$  would be needed to explain the observed energy production.

TABLE VII.  $p-\alpha$  reactions.

INITIAL NUCLEUS	PRODUCT NUCLEUS	ENERGY EVOLUTION Q (MMU)	POTENTIAL BARRIER B (MMU)	PENETRABILITY P
Li <sup>6</sup>	He <sup>3</sup>	4.14		1
Li <sup>7</sup>	He <sup>4</sup>	18.59		1
Be <sup>9</sup>	Li <sup>6</sup>	2.45	2.6	1
Be <sup>10</sup>	Be <sup>7</sup>	1.2	3.4	0.027
Be <sup>11</sup>	2He <sup>4</sup>	9.4		1
C <sup>12</sup>	B <sup>9</sup>	-8.1		0
C <sup>13</sup>	B <sup>10</sup>	-4.4		0
N <sup>14</sup>	C <sup>11</sup>	-3.5		0
N <sup>15</sup>	C <sup>12</sup>	5.2	4.6	1
O <sup>16</sup>	N <sup>13</sup>	-5.8		0
O <sup>17</sup>	N <sup>14</sup>	1.3	5.1	$1.7 \cdot 10^{-4}$
O <sup>18</sup>	N <sup>15</sup>	3.1	5.0	0.2
F <sup>19</sup>	O <sup>16</sup>	8.8		1
Ne <sup>20</sup>	F <sup>17</sup>	-4.5		0
Ne <sup>21</sup>	F <sup>18</sup>	-1.6		0
Ne <sup>22</sup>	F <sup>19</sup>	-1.6		0
Na <sup>23</sup>	Ne <sup>20</sup>	1.6	6.7	$6 \cdot 10^{-6}$
Mg <sup>24</sup>	Na <sup>21</sup>	< -3.0		0
Mg <sup>25</sup>	Na <sup>22</sup>	-2.1		0
Mg <sup>26</sup>	Na <sup>23</sup>	-2.0		0
Al <sup>27</sup>	Mg <sup>24</sup>	1.8	7.6	$1.1 \cdot 10^{-6}$
Si <sup>28</sup>	Al <sup>25</sup>	< -2.9		0
Si <sup>29</sup>	Al <sup>26</sup>	-2.0		0
Si <sup>30</sup>	Al <sup>27</sup>	-2.4		0
P <sup>31</sup>	Si <sup>28</sup>	2.0	8.5	$2.5 \cdot 10^{-7}$
S <sup>32</sup>	P <sup>29</sup>	< 0		0
S <sup>33</sup>	P <sup>30</sup>	-2		0
S <sup>34</sup>	P <sup>31</sup>	-2.0		0
Cl <sup>35</sup>	S <sup>32</sup>	2.3	9.3	$5 \cdot 10^{-8}$
Cl <sup>37</sup>	S <sup>34</sup>	4.2	9.1	$2.5 \cdot 10^{-9}$

assumption of a N<sup>14</sup> concentration of 10 percent by weight, this gives an energy evolution of

$$\frac{6 \cdot 10^{23} \cdot 0.1}{14} \cdot 3 \cdot 10^{-20} \approx 100 \text{ ergs/g sec.} \quad (45)$$

at "standard stellar conditions," i.e.,  $T = 2 \cdot 10^7$ ,  $\rho = 80$ , hydrogen concentration 35 percent.

This result is just about what is necessary to explain the observed luminosity of the sun. Since the nitrogen reaction depends strongly on the temperature (as  $T^{18}$ ) and the temperature, as well as the density, decrease rapidly from the center of the sun outwards, the average energy production will be only a fraction, perhaps 1/10 to 1/20, of the production at the center.<sup>36b</sup> This means that the average production is 5 to 10 ergs/g sec., in excellent agreement with the observed luminosity of 2 ergs/g sec.

<sup>36b</sup> *Added in proof.*—According to calculations of R. Marshak, the correct figure is about 1/30.

Thus we see that the reaction between nitrogen and protons which we have recognized as the logical reaction for energy production from the point of view of nuclear physics, also agrees perfectly with the observed energy production in the sun. This result can be viewed from another angle: We may ignore, for the moment, all our nuclear considerations and ask simply which nucleus will give us the right energy evolution in the sun? Or conversely: Given an energy evolution of 20 ergs/g sec. at the center of the sun, which nuclear reaction will give us the right central temperature ( $\sim 19 \cdot 10^6$  degrees)?

This calculation has been carried out in Table VI. It has been assumed that the density is 80, the hydrogen concentration 35 percent and the concentration of the other reactant 10 percent by weight. The "widths" were assumed the same as in Table V. Given are the necessary temperatures for an energy production of 20 ergs/g sec. It is seen that all nuclei up to boron require extremely low temperatures in order not to give too much energy production; these temperatures ( $< 10^7$  degrees) are quite irreconcilable with the equations of hydrostatic and radiation equilibrium. On the other hand, oxygen and neon would require much too high temperatures. Only carbon and nitrogen require nearly, and nitrogen in fact exactly, the central temperature obtained from the Eddington integrations ( $19 \cdot 10^6$  degrees). Thus from stellar data alone we could have predicted that the capture of protons by N<sup>14</sup> is the process responsible for the energy production.

## §8. REACTIONS WITH HEAVIER NUCLEI

Mainly for the sake of completeness, we shall discuss briefly the reactions of nuclei heavier than nitrogen. For the energy production, these reactions are obviously of no importance because the higher potential barrier of the heavier nuclei makes their reactions much less probable than those of the carbon-nitrogen group.

The most important point for a qualitative discussion is the question whether a  $p-\alpha$  reaction is energetically possible for a particular nucleus, and, if possible, whether it is impeded by the potential barrier. In Table VII are listed the energy evolution in  $p-\alpha$  reactions for all stable

(nonradioactive) nuclei up to chlorine. In the first column, the reacting nucleus is given, in the second, the product of a  $p-\alpha$  reaction. The third column contains the reaction energy  $Q$ ; when  $Q$  is negative, the reaction is energetically impossible so that the initial nucleus can only capture protons with  $\gamma$ -emission. In the fourth column, the height of the nuclear potential barrier is given for all reactions with positive  $Q$ . In the last column, the penetrability of the potential barrier is calculated according to standard methods (reference 10, p. 166). If  $Q > B$ , the penetrability is 1; if  $Q$  is negative,  $P=0$  was inserted.

The *a priori* probability of a  $p-\alpha$  reaction is roughly  $10^4$  times that of radiative capture. Therefore the emission of  $\alpha$ -particles will be preferred when  $P > 10^{-4}$ . It is seen from the table that for all nuclei up to boron the  $p-\alpha$  reaction is strongly preferred, a fact which we recognized as the main reason for the impossibility of building up heavier elements than He<sup>4</sup> (§5). Furthermore, in the carbon group, only proton capture is possible for C<sup>12</sup>C<sup>13</sup>N<sup>14</sup> while for N<sup>15</sup> the  $p-\alpha$  reaction will strongly predominate (cf. §7).

The oxygen-fluorine group shows intermediate behavior. O<sup>16</sup> can only capture protons, for O<sup>17</sup> the capture and the  $\alpha$ -emission will have roughly equal probability while for O<sup>18</sup> and F<sup>19</sup> the  $p-\alpha$  reaction will be much more probable. With a ratio  $10^4$  for the *a priori* probabilities, about 40 percent of the O<sup>17</sup> will become F<sup>18</sup> (and then O<sup>18</sup> by positron emission) while 60 percent will revert to N<sup>14</sup>. Of the O<sup>18</sup>, only 1 part in 2000 will become F<sup>19</sup>, and of the F<sup>19</sup>, only 1 in 10,000 will transform into Ne<sup>20</sup>. Thus, under continued proton bombardment, about one O<sup>16</sup> nucleus in  $5 \cdot 10^7$  will ultimately transform into Ne<sup>20</sup>, the rest will become nitrogen.

Actually, these considerations are somewhat academic because in general the supply of protons will be exhausted long before all the O<sup>16</sup> initially present in the star will have captured a proton. Because of the small energy evolution in the reaction O<sup>16</sup>+H=F<sup>17</sup>, this reaction is extremely slow ( $\sim 10^{12}$  years) so that equilibrium in the oxygen group will not be reached in astronomical times.

Among the nuclei heavier than fluorine, the  $p-\alpha$  reaction is in general energetically permitted only for those with mass number  $4n+3$ . But even for these, the energy evolution is so much less than the height of the barrier that the penetrabilities are extremely small. Thus for all these elements only proton capture will occur (with the possible exception of Cl<sup>37</sup>).

These considerations demonstrate the uniqueness of the carbon-nitrogen cycle.

### §9. AGREEMENT WITH OBSERVATIONS

In Table VIII, we have made a comparison of our theory (carbon-nitrogen reaction) with observational data for five stars for which such data are given by Strömgren.<sup>1</sup> The first five columns are taken from his table, the last contains the necessary central temperature to give the correct energy evolution with the carbon-nitrogen reactions (cf. Table VI). As in §7, we have assumed a N<sup>14</sup> content of 10 percent, and an energy production at the center of ten times the average energy production (listed in the second column).

The result is highly satisfactory: The temperatures necessary to give the correct energy evolution (last column) agree very closely with the temperatures obtained from the Eddington integration (second last column). The only exception from this agreement is the giant Capella: This is not surprising because this star has greater luminosity than the sun at smaller density and temperature; such a behavior cannot possibly be explained by the same mechanism which ac-

TABLE VIII. Comparison of the carbon-nitrogen reaction with observations.

STAR	LUMINOSITY ERG/G SEC.	CENTRAL DENSITY	$H$ CONTENT (PER- CENT)	CENTRAL TEM- PERATURE (MILLION DEGREES)	
				INTE- GRATION	ENERGY PRODUC- TION
Sun	2.0	76	35	19	18.5
Sirius A	30	41	35	26	22
Capella	50	0.16	35	6	32
U Ophiuchi (bright)	180	12	50	25	26
Y Cygni (bright)	1200	6.5	80	32	30

<sup>17</sup> A. S. Eddington, *The Internal Constitution of the Stars* (Cambridge University Press, 1926).

counts for the main sequence. We shall come back to the problem of energy production in giants at the end of this section.

For the main sequence we observe that the small increase of central temperature from the sun to Y Cygni (19 to  $33 \cdot 10^6$  degrees) is sufficient to explain the much greater energy production ( $10^4$  times) of the latter. The reason for this is, of course, the *strong temperature dependence of our reactions* ( $\sim T^{18}$ , cf. §10). We may say that *astrophysical data themselves would demand such a strong dependence* even if we did not know that the source of energy are nuclear reactions. The small deviations in Table VIII can, of course, easily be attributed to fluctuations in the nitrogen content, opacity, etc.

In judging the agreement obtained, it should be noted that the "observational" data in Table VIII were obtained by integration of an Eddington model,<sup>37</sup> i.e., the energy production was assumed to be almost constant throughout the star. Since our processes are strongly temperature dependent, the "point source" model should be a much better approximation. However, it seems that the results of the two models are not very different so that the Eddington model may suffice until accurate integrations with the point source model are available.<sup>37a</sup>

Since our theory gives a definite mechanism of energy production, it permits decisions on questions which have been left unanswered by astrophysicists for lack of such a mechanism. The first is the question of the "model," which is answered in favor of one approximating a point source model. The second is the problem of chemical composition. The equilibrium conditions permit for the sun a hydrogen content of either 35 or 99.5 percent when there is no helium, and intermediate values when there is helium. The central temperature varies from  $19 \cdot 10^6$  to  $9.5 \cdot 10^6$  when the hydrogen content increases

<sup>37a</sup> Mr. Marshak has kindly calculated the central temperature and density of the sun for the point source model, using Strömgren's tables for which we are indebted to Professor Strömgren. With an average atomic weight  $\mu = 1$ , Marshak finds

for the point source model  $T_c = 20.3 \cdot 10^6$ ,  $\rho_c = 50.2$   
for the Eddington model  $T_c = 19.6 \cdot 10^6$ ,  $\rho_c = 72.2$

Not only is the temperature difference very small ( $3\frac{1}{2}$  percent) but it is, for the sake of the energy production, almost compensated by a density difference in the opposite direction. The product  $\rho_c T_c^{18}$  is only 20 percent greater for the point source model.

from 35 to 99.5 percent. It is obvious that the latter value can be definitely excluded on the basis of our theory: The energy production due to the carbon-nitrogen reaction would be reduced by a factor of about  $10^8$  (100 for nitrogen concentration,  $10^6$  for temperature). The proton combination (1) would still supply about 5 percent of the observed luminosity; but apart from the fact that a factor 20 is missing, the proton combination does not depend sufficiently on temperature to explain the larger energy production in brighter stars of the main sequence. Thus it seems that only a small range of hydrogen concentrations around 35 percent is permitted; what this range is, depends to some extent on the  $N^{14}$  concentration and also requires a more accurate determination of the distribution of temperature and density.

Next, we want to point out a rather well-known difficulty about the energy production of very heavy stars such as Y Cygni. With an energy production of 1200 ergs/g sec., and an available energy of  $1.0 \cdot 10^{-5}$  erg per proton (formation of  $\alpha$ -particles!), all the energy will be consumed in  $1.7 \cdot 10^8$  years. Since at present Y Cygni still has a hydrogen content of 80 percent, its past life should be less than  $3.5 \cdot 10^7$  years. We must therefore conclude that Y Cygni and other heavy stars were "born" comparatively recently—by what process, we cannot say. This difficulty, however, is not peculiar to our theory of stellar energy production but is inherent in the well-founded assumption that nuclear reactions are responsible for the energy production.<sup>38</sup>

Finally, we want to come back to the problem of stars outside the main sequence. The white dwarfs presumably offer no great difficulty. The internal temperature of these stars is probably rather low,<sup>1, 39</sup> because of the low opacity (degeneracy!) so that the small energy production may be understandable. Quantitative calculations are, of course, necessary. For the giants, on the other hand, it seems to be rather difficult to account for the large energy production by nuclear reactions. If the Eddington (or the point

<sup>38</sup> Even if the most stable nuclei (Fe, etc.) are formed rather than He, the possible life will only increase by 30 percent.

<sup>39</sup> S. Chandrasekhar, Monthly Not. 95, 207, 226, 676 (1935).

## ENERGY PRODUCTION IN STARS

TABLE IX. Relations between stellar constants.

QUANTITY	$\gamma = 18$ $\alpha = \frac{1}{16}$ $\beta = 2\frac{1}{4}$ $\delta = 19\frac{1}{4}$	$\gamma = 18$ $\alpha = 1$ $\beta = 3\frac{1}{2}$ $\delta = 20\frac{1}{4}$	$\gamma = 15$ $\alpha = \frac{1}{16}$ $\beta = 2\frac{1}{4}$ $\delta = 16\frac{1}{4}$	$\gamma = 4.5$ $\alpha = \frac{1}{16}$ $\beta = 2\frac{1}{4}$ $\delta = 6\frac{1}{4}$
Radius $R$	$M^{0.75} \mu^{0.57} (yz)^{0.05}$	$M^{0.71} \mu^{0.51} (yz)^{0.05}$	$M^{0.70} \mu^{0.49} (yz)^{0.06}$	$M^{0.20} \mu^{-0.38} (yz)^{0.18}$
Temperature $T$	$M^{0.24} \mu^{0.43} (yz)^{-0.05}$	$M^{0.29} \mu^{0.49} (yz)^{-0.05}$	$M^{0.40} \mu^{0.51} (yz)^{-0.06}$	$M^{0.80} \mu^{1.36} (yz)^{-0.16}$
Density $\rho$	$M^{-1.25} \mu^{-1.71} (yz)^{-0.15}$	$M^{-1.13} \mu^{-1.63} (yz)^{-0.15}$	$M^{-1.10} \mu^{-1.47} (yz)^{-0.18}$	$M^{0.40} \mu^{1.08} (yz)^{-0.48}$
Luminosity $L$	$M^{4.22} \mu^{6.04} y^{-1.02} z^{-0.06}$	$M^{3.18} \mu^{7.24} y^{-1.02} z^{-0.02}$	$M^{4.37} \mu^{6.15} y^{-1.07} z^{-0.07}$	$M^{3.00} \mu^{7.20} y^{-1.20} z^{-0.20}$
Surf. temp. $T_s$	$M^{0.70} \mu^{1.22} y^{-0.29} z^{-0.04}$	$M^{0.93} \mu^{1.55} y^{-0.28} z^{-0.03}$	$M^{0.74} \mu^{1.29} y^{-0.30} z^{-0.05}$	$M^{1.25} \mu^{1.98} y^{-0.38} z^{-0.12}$

source) model is used, the central temperatures and densities are exceedingly low, e.g., for Capella  $T=6 \cdot 10^6$ ,  $\rho=0.16$ . Only a nuclear reaction going at very low temperature is therefore at all possible;  $\text{Li}^7 + \text{H} = 2\text{He}^4$  would be just sufficient. But it seems difficult to conceive how the  $\text{Li}^7$  should have originated in *all* the giants in the first place, and why it was not burned up long ago. The only other source of energy known is gravitation, which would require a core model<sup>40</sup> for giants.<sup>41</sup> However, any core model seems to give small rather than large stellar radii.

#### §10. THE MASS-LUMINOSITY RELATION

In this section, we shall use our theory of energy production to derive the relation between mass and luminosity of a star. For this purpose, we shall employ the well-known homology relations (reference 1, p. 492). This is justified because we assume that all stars have the same mechanism of energy evolution and therefore follow the same model. Further, it is assumed that the matter throughout the star is non-degenerate which seems to be true for all stars except the white dwarfs. (For all considerations in this and the following two sections, cf. reference 1.)

We shall consider the mass of the star  $M$ , the mean molecular weight  $\mu$ , the concentration of "Russell Mixture"  $y$  and the product of the concentrations of hydrogen and nitrogen,  $z$ , as independent variables. In addition, we introduce for the moment the radius  $R$  which, however, will be eliminated later. Then, obviously, we have for the density (at each point)

$$\rho \sim M/R^3. \quad (46)$$

<sup>40</sup> L. Landau, Nature 141, 333 (1938).

<sup>41</sup> This suggestion was made by Gamow in a letter to the author.

From the equation of hydrostatic equilibrium

$$dp/dr = -GM\rho/r^2 \quad (47)$$

( $G$ =gravitational constant) and the gas equation

$$p = RT\rho/\mu \quad (47a)$$

( $R$  the gas constant, radiation pressure neglected), we find

$$T \sim M\mu/R. \quad (48)$$

Finally, we must use the equation of radiative equilibrium:

$$aT^3 \frac{dT}{dr} = -\frac{3k}{4c} \rho \frac{L_r}{4\pi r^2}, \quad (49)$$

where  $a$  is the Stefan-Boltzmann constant,  $c$  the velocity of light,  $k$  the opacity, and  $L_r$  the luminosity (energy flux) at distance  $r$  from the center.

For the opacity, we assume

$$k \sim y\rho^\alpha T^\beta \quad (50)$$

( $y$  concentration of heavy elements). Usually,  $\alpha$  is taken as 1 and  $\beta=3.5$  (Kramers' formula). However, the Kramers formula must be divided by the "guillotine factor"  $\tau$  which was calculated from quantum mechanics by Strömgren.<sup>42</sup> For densities between 10 and 100, and temperatures between  $10^7$  and  $3 \cdot 10^7$ , Strömgren's numerical results can be fairly well represented by taking  $\tau \sim \rho^{\frac{1}{3}} T^{-1}$ . Therefore we adopt  $\alpha=\frac{1}{2}$ ,  $\beta=2.75$  in (50).

The luminosity may be written

$$L \sim M\rho z T^\gamma. \quad (51)$$

That the energy production per unit mass,  $L/M$ , contains a factor  $\rho$  follows from the fact that it is due to two-body nuclear reactions; this factor is

<sup>42</sup> Cf. reference 1, Table 6, p. 485.

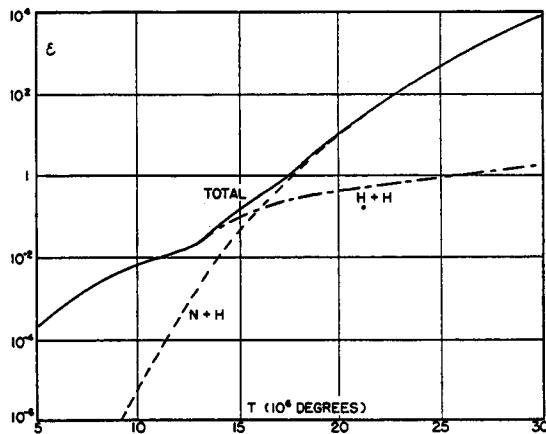


FIG. 1. The energy production in ergs/g sec. due to the proton-proton combination (curve  $H+H$ ) and the carbon-nitrogen cycle ( $N+H$ ), as a function of the central temperature of the star. Solid curve: total energy production caused by both reactions. The following assumptions were made: central density = 100, hydrogen concentration 35 percent, nitrogen 10 percent; average energy production 1/5 of central production for  $H+H$ , 1/10 for  $N+H$ .

apparent from all our formulae, e.g., (4).  $z = x_1 x_2$  is the product of the concentrations of the reacting nuclei ( $N^{14}$  and H). For  $\gamma$  we obtain from (4), (6)

$$\gamma = \frac{d \log (\tau^2 e^{-\tau})}{d \log T} = \frac{1}{3}(\tau - 2). \quad (52)$$

For  $N^{14} + H$  and  $T = 2 \cdot 10^7$ , this gives  $\gamma = 18$ . For  $T = 3.2 \cdot 10^7$  (Y Cygni),  $\gamma = 15.5$ ; generally,  $\gamma \sim T^{-1}$ .  $\gamma = 18$  will be a good approximation over most of the main sequence.

Inserting (50), (51) in (49), we have

$$T^{4+\beta-\gamma} \sim yz M \rho^{2+\alpha} R^{-1}. \quad (53)$$

Combining this with (46), (48), and introducing the abbreviation

$$\delta = \gamma + 3 + 3\alpha - \beta \quad (54)$$

we find

$$R \sim M^{1-2(2+\alpha)/\delta} \mu^{1-(7+3\alpha)/\delta} (yz)^{1/\delta}, \quad (55)$$

$$T \sim M^{2(2+\alpha)/\delta} \mu^{(7+3\alpha)/\delta} (yz)^{-1/\delta}, \quad (56)$$

$$\rho \sim M^{-2+6(2+\alpha)/\delta} \mu^{-3+3(7+3\alpha)/\delta} (yz)^{-3/\delta}, \quad (57)$$

$$L \sim M^{3+2\alpha+2(2+\alpha)(\beta-3\alpha)/\delta} \mu^{4+3\alpha+(7+3\alpha)(\beta-3\alpha)/\delta} \\ \times y^{-1} (yz)^{-(\beta-3\alpha)/\delta}. \quad (58)$$

Furthermore, the surface temperature may be of

interest, we have

$$T_s \sim L^{\frac{1}{3}} R^{-\frac{1}{3}} \sim M^{\frac{1}{3} + \frac{1}{3}\alpha + \frac{1}{3}(2+\alpha)(\beta-3\alpha+2)/\delta} \\ \times \mu^{\frac{1}{3} + \frac{1}{3}\alpha + \frac{1}{3}(7+3\alpha)(\beta-3\alpha+2)/\delta} y^{-\frac{1}{3}} \\ \times (yz)^{-\frac{1}{3}(\beta-3\alpha+2)/\delta}. \quad (59)$$

In Table IX, these formulas are given explicitly, for four different sets of constants.

The most important result is that the central *temperature* depends only slightly on the mass of the star, *viz.* as  $M^{0.25}$  and  $M^{0.30}$  for  $\gamma = 18$  and 15. The reason for this is the strong temperature dependence of the reaction rate: The exponent of  $M$  in (56) is inversely proportional to  $\delta$  which is mainly determined (cf. (54)) by the exponent  $\gamma$  in formula (51) for the temperature dependence of the reaction rate. The integration of the Eddington equations with the use of observed luminosities, radii, etc., gives, in fact, only a small dependence of the central temperature on the mass. This can *only* be explained by a strong temperature dependence of the source of stellar energy, a fact which has not been sufficiently realized in the past. Theoretically, the central temperature increases somewhat with increasing mass of the star, more strongly with the mean molecular weight, and is practically independent of the chemical composition, i.e., of  $y$  and  $z$ .

The *radius* of the star is larger for heavy stars and for high molecular weight. The density behaves, of course, in the opposite way. Both these results are in qualitative agreement with observation. The product of mass and density which occurs in Eq. (51) for the luminosity, is almost independent of the mass; therefore, for constant concentrations  $z$ , the luminosity is determined by the central temperature alone. Both radius and density are almost independent of the chemical composition, except insofar as it affects  $\mu$ .

The *luminosity* increases slightly faster than the fourth power of the mass and the sixth power of the mean molecular weight. This increase is considerably less than that usually given ( $M^{4.5} \mu^{7.5}$ ) and agrees better with observation. The difference from the usual formula is mainly due to the different dependence of the opacity on density and temperature; in fact, with the usual assumption ( $\alpha = 1$ ,  $\beta = 3\frac{1}{2}$ ), we obtain  $M^{5.15} \mu^{7.24}$ .

The remaining difference is that the dependence on the radius is carried as a separate factor in the usual formula while we have expressed  $R$  in terms of  $M$  and  $\mu$ . The observations show, for bright stars, an even slower increase than  $M^4$ ; this seems to be due to the lower average molecular weight (higher hydrogen content) of most very bright stars. It may be that these stars become unstable because of excessive energy production when their hydrogen content becomes too low (cf. §12).—The luminosity is inversely proportional to the concentration  $y$  of heavy elements (Russell mixture) because  $y$  determines the opacity. However,  $L$  is almost independent of the nitrogen concentration, as are  $R$ ,  $T$  and  $\rho$ .

All these considerations are valid for bright stars, down to about three magnitudes fainter than the sun. For fainter stars, with lower central temperatures, the proton combination  $H+H = D + \epsilon^+$  should become more probable than the carbon-nitrogen reactions, because this reaction depends less on temperature. In discussing the energy production from  $H+H$ , we must take into account that (cf. §5) at low temperatures, this reaction leads only to  $He^3$  rather than  $He^4$ , because of the slowness of the reaction  $He^4 + He^3 = Be^7$ . (Assumption B of §5 is made, *viz.* that  $He^3$  is more stable than  $H^3$ , and  $Li^4$  unstable.) This causes a rather sudden drop in the energy evolution from  $H+H$  around  $14 \cdot 10^6$  degrees (cf. Fig. 1), i.e., just below the temperature at which the proton combination becomes important ( $\sim 16 \cdot 10^6$  degrees, see Fig. 1). Therefore, the temperature exponent  $\gamma$  stays fairly large ( $\sim 13$ , cf. Fig. 2) down to about  $13 \cdot 10^6$  degrees which corresponds to an energy production of about one percent of that of the sun (five magnitudes fainter). For still fainter stars,  $\gamma$  drops to very low values, reaching a minimum of about 4.5 near  $10^7$  degrees.

The relations between central temperature, radius, luminosity and mass for this case ( $\gamma=4.5$ ) are given in the last column of Table IX. The temperature is seen to depend much more strongly on the mass (as  $M^{0.80}$ ) while the radius becomes almost independent of  $M$  and the density decreases with decreasing mass. The luminosity decreases faster with the mass (as  $M^5$ ) than for the bright stars. Unfortunately, little material is available for these fainter stars. This

is the more regrettable as it is rather important for nuclear physics to decide whether the  $H+H$  reaction is really as probable as assumed in this paper: There is some possibility that it is forbidden by selection rules (cf. reference 16, p. 250) in which case it would be about  $10^6$  times less probable. Then the carbon-nitrogen reactions would furnish the energy even for faint stars, and the central temperature of these stars would not depend much on their mass.

Figure 1 gives the energy production due to the proton combination ( $H+H$ ) and to the carbon-nitrogen reactions ( $N+H$ ) as a function of the central temperature, on a logarithmic scale. The great preponderance of  $H+H$  at low and  $N+H$  at high temperatures is evident. The following assumptions were made: Hydrogen concentration 35 percent, nitrogen 10 percent, central density  $\rho=100$ , average energy production =  $\frac{1}{2}$  of central production for  $H+H$ ,  $\frac{1}{10}$  for  $N+H$  reaction.  $He^3$  is supposed to be more stable than  $H^3$ , and  $Li^4$  unstable (assumption B of §5).

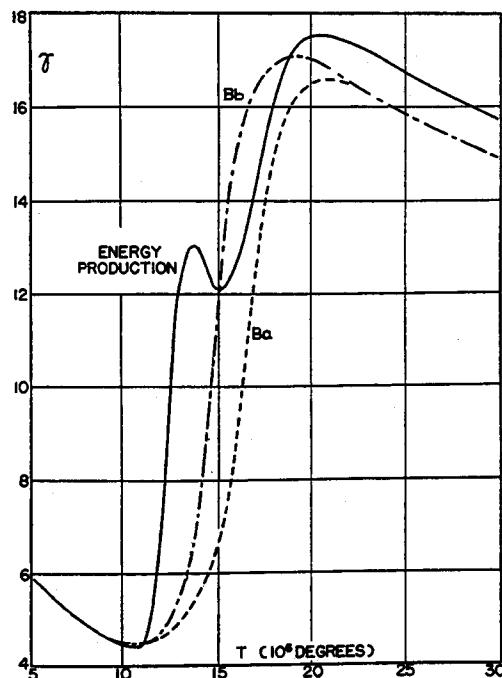


FIG. 2. The exponent  $\gamma$  in the relation  $L \sim T^\gamma$  between luminosity  $L$  and temperature  $T$ , as a function of  $T$ . Solid curve:  $\gamma$  for total energy production (logarithmic derivative of solid curve in Fig. 1). Dotted curves:  $\gamma$  for stability against temperature changes (curve Ba for times less than 14 months. Bb for more than 14 months).

Figure 2, solid curve, gives the exponent  $\gamma$  in the *total* energy production. It is low at low temperatures ( $\sim 4\text{--}5$ , hydrogen reaction) and has a minimum of 4.44 at 11 million degrees. Between 11 and 14 million degrees,  $\gamma$  rises steeply as the reaction  $\text{He}^4 + \text{He}^3 = \text{Be}^7$  sets in (§5); then it falls again from 13 to 12 when this reaction reaches saturation. From  $T=15$ , the carbon-nitrogen reactions set in, causing a rise of  $\gamma$  to a maximum of 17.5 at  $T=20$ , while at higher temperatures  $\gamma$  decreases again as  $T^{-\frac{1}{4}}$ .

### §11. STABILITY AGAINST TEMPERATURE CHANGES

Cowling<sup>48</sup> has investigated the stability of stars against vibration. This stability is determined mostly by the ratio  $\gamma$  of the specific heats at constant pressure and constant volume. If the radiation pressure in the star is negligible compared with the gas pressure ( $\gamma=5/3$ ) then the star will be stable for any value of the temperature exponent  $n$  in the energy production (38), up to  $n \approx 450$ . Only for very heavy stars, for which the radiation pressure is comparable with the gas pressure, does the stability condition put a serious restriction on the temperature dependence of the energy production. According to our theory, the energy production is proportional to  $T^{17}$  (see below); according to Cowling, stability will then occur when  $\gamma > 10/7$ . The corresponding ratio of radiation pressure to total pressure is

$$1 - \beta = \frac{5 - 3\gamma}{3(7\gamma - 9)} = 0.24 \quad (60)$$

and the corresponding mass of the star, according to Eddington's "standard model," is  $17/\mu^2 \odot$ , where  $\mu$  is the average molecular weight. Therefore practically all the stars for which good observational data are available will be stable.

It may be worth while to point out that the temperature exponent  $n$  for these stability considerations is not exactly equal to that for the energy production in equilibrium. A change of temperature gives rise to radial vibrations of the star whose period is of the order of days or, at most, a few years. On the other hand, when the temperature is raised or lowered, the equilibrium

between carbon and nitrogen will be disturbed and it takes a time of the order of the lifetime of  $\text{C}^{12}$  ( $\sim 10^6$  years) to restore equilibrium at the new temperature. Thus we must take the concentrations of carbon and nitrogen corresponding to the *original* temperature.

At  $T=2 \cdot 10^7$  degrees, the carbon reactions have a  $\tau=50.6$  (Table V) and therefore a temperature exponent  $\gamma_C=16.2$  (cf. 52); the nitrogen reactions have  $\tau=56.3$  and  $\gamma_N=18.1$ . The number of reactions per second is, in equilibrium, the same for each of the reactions in the chain (42). The energy evolution in the first three reactions together is 11.7 mMU, after subtracting 0.8<sub>8</sub> mMU for the neutrino emitted by  $\text{N}^{13}$ . These three reactions are carbon reactions, the remaining three, with an energy evolution of 15.0 mMU, are nitrogen reactions. Thus the effective temperature exponent for stability problems becomes

$$\gamma = \frac{11.7\gamma_C + 15.0\gamma_N}{26.7} = 17.3 \quad (60a)$$

at  $2 \cdot 10^7$  degrees.  $\gamma$  is approximately proportional to  $T^{-\frac{1}{4}}$  (cf. 52, 6).

For the proton combination, we have to distinguish the three possibilities discussed in §5. The simplest of these is assumption C.

#### Assumption C: $\text{Li}^4$ unstable, $\text{H}^3$ more stable than $\text{He}^3$

In this case, there are two "slow" processes, *viz.* (a) the original reaction  $\text{H}+\text{H}$  and (b) the transformation of  $\text{He}^3$  into  $\text{H}^3$  by electron capture ( $\sim 2000$  years). (a) depends on temperature approximately as  $T^{3.5}$ , (b) is independent of  $T$ . The energy evolution up to the formation of  $\text{He}^3$  is 7.2 mMU, from  $\text{He}^3$  to  $\text{He}^4$  21.3 mMU. Thus

$$\gamma = \frac{7.2 \cdot 3.5 + 21.3 \cdot 0}{28.5} = 0.9. \quad (61C)$$

This would be a very slight dependence indeed.

#### Assumption A: $\text{Li}^4$ stable

According to Table V, the transformation of  $\text{He}^3$  into  $\text{Li}^4$  takes about one day.

(a) For times shorter than one day, the reactions up to  $\text{He}^3$  and from then on are independent of each other. The first group again has  $\gamma_H=3.5$  and gives 7.2 mMU, the second group now gives only 8.3 mMU because the remaining 13.0 are lost to the neutrino from  $\text{Li}^4$  (cf. §5) and has (Table V)  $\gamma_{\text{He}^4}=6.9$ . Therefore

$$\gamma = \frac{7.2 \cdot 3.5 + 8.3 \cdot 6.9}{15.5} = 5.3. \quad (61Aa)$$

<sup>48</sup> T. G. Cowling, Monthly Not. 94, 768 (1934); 96, 42 (1935).

(b) For times *longer than one day*, the proton combination determines the whole chain of reactions so that

$$\gamma = 3.5. \quad (61\text{Ab})$$

**Assumption B.** Li<sup>4</sup> unstable, He<sup>3</sup> more stable than H<sup>3</sup> (most probable assumption)

As was pointed out in §5, the reaction He<sup>4</sup>+He<sup>3</sup>=Be<sup>7</sup> is so slow ( $3 \cdot 10^7$  years, Table V) that the concentration of He<sup>3</sup> will remain unaffected by the temperature fluctuation. Be<sup>7</sup> has a mean life of 14 months at the center of the sun so that there are again two cases:

(a) *For times less than 14 months*, there are three groups of reactions, (a) those up to He<sup>3</sup>, giving again 7.2 mMU with  $\gamma_H = 3.5$ , (b) the reaction He<sup>4</sup>+He<sup>3</sup>=Be<sup>7</sup>, giving (Table V) 1.6 mMU with  $\gamma_{H_0} = 15.1$ , and (c) the electron capture by Be<sup>7</sup>, followed by Li<sup>7</sup>+H=2He<sup>4</sup>. This last reaction does not depend on temperature ( $\gamma_{B_0} = 0$ ) and gives 18.6 mMU. Therefore the effective  $\gamma$  becomes

$$\gamma = \frac{7.2 \cdot 3.5 + 1.6 \cdot 15.1 + 18.6 \cdot 0}{27.4} = 1.8. \quad (61\text{Ba})$$

(b) *For times longer than 14 months*, the reaction He<sup>4</sup>+He<sup>3</sup>=Be<sup>7</sup> governs all the energy evolution from He<sup>3</sup> on, so that

$$\gamma = \frac{7.2 \cdot 3.5 + 20.2 \cdot 15.1}{27.4} = 12.1 \quad (61\text{Bb})$$

at  $2 \cdot 10^7$  degrees.

At low temperatures, the reaction He<sup>4</sup>+He<sup>3</sup>=Be<sup>7</sup> stops altogether (cf. §5) so that then the  $\gamma$  of the H+H reaction itself determines the radial stability. From  $12$  to  $16 \cdot 10^6$  degrees we have a transition region in which the importance of the He<sup>4</sup>+He<sup>3</sup> reaction (and the consequent ones) is reduced.

In Fig. 2, curves Ba and Bb, we have plotted the effective  $\gamma$  for the radial stability, by taking into account both C+N and H+H reactions, and making the same assumptions about the concentrations of hydrogen and nitrogen as in Fig. 1 (cf. end of §10). Assumption B was made regarding the stability of Li<sup>4</sup> and He<sup>3</sup>; the curves Ba and Bb refer to the short time and long time formulas (61Ba) and (61Bb). At high temperatures, the two curves coincide because

then the proton combination is unimportant compared with the carbon-nitrogen reactions. The combined  $\gamma$  is seen to reach a maximum of 17 (for the long time curve).

## §12. STELLAR EVOLUTION<sup>44</sup>

We have shown that the concentrations of heavy nuclei (Russell mixture) and, therefore, also of nitrogen, cannot change appreciably during the life of a star. The only process that occurs is the transformation of hydrogen into helium, regardless of the detailed mechanism. The state of a star is thus described by the hydrogen concentration  $x$ , and by a *fixed* parameter,  $y$ , giving the concentration of Russell mixture. The rest,  $1-x-y$ , is the helium concentration. Without loss of generality, we may fix the zero of time so that the helium concentration is zero. (Then the actual "birth" of the star may occur at  $t > 0$ ).

It has been shown (Table IX) that the luminosity depends on the chemical composition practically only<sup>45</sup> through the mean molecular weight  $\mu$ . This quantity is given by

$$1/\mu = 2x + \frac{3}{4}(1-x-y) + \frac{1}{2}y = (5/4)(x+a), \quad (62)$$

$$a = 0.6 - 0.2y, \quad (62\text{a})$$

taking for the molecular weights of hydrogen, helium and Russell mixture the values  $\frac{1}{2}$ ,  $4/3$  and 2, respectively.<sup>46</sup>

Now the rate of decrease of the hydrogen concentration is proportional to the luminosity, which we put proportional to  $\mu^n$ . According to Table IX,  $n$  is about 6. Then

$$dx/dt \sim -(x+a)^{-n}. \quad (63)$$

Integration gives

$$(x+a)^{n+1} = A(t_0 - t), \quad (64)$$

where  $A$  is a constant depending on the mass and other characteristics of the star. Since  $x=1-y$  at  $t=0$ , we have

$$At_0 = (1.6 - 1.2y)^{n+1}. \quad (64\text{a})$$

<sup>44</sup> Most of these considerations have already been given by G. Gamow, Phys. Rev. 54, 480(L) (1938).

<sup>45</sup> Except for the factor  $y^{-1}$  which, however, does not change with time.

It is obvious from (63) and (64) that the hydrogen concentration decreases slowly at first, then more and more rapidly. E.g., when the concentration of heavy elements is  $y = \frac{1}{2}$ , the first half of the hydrogen in the star will be consumed in 87 percent of its life, the second half in the remaining 13 percent. If the concentration of Russell mixture is small, the result will be even more extreme: For  $y = 0$ , it takes 92 percent of the life of the star to burn up the first half of the hydrogen. Consequently, very few stars will actually be found near the end of their lives even if the age of the stars is comparable with their total lifespan  $t_0$  (cf. 64a). In reality, the lifespan of all stars, except the most brilliant ones, is long compared with the age of the universe as deduced from the red-shift ( $\sim 2 \cdot 10^9$  years): E.g., for the sun, only one percent of the total mass transforms from hydrogen into helium every  $10^9$  years so that there would be only 2 percent He in the sun now, provided there was none "in the beginning." The prospective future life of the sun should according to this be  $12 \cdot 10^9$  years.

It seems to us that this comparative youth of the stars is one important reason for the existence of a *mass-luminosity* relation—if the chemical composition, and especially the hydrogen content, could vary absolutely at random we should find a greater variability of the luminosity for a *given mass*.

It is very interesting to ask what will happen to a star when its hydrogen is almost exhausted. Then, obviously, the energy production can no longer keep pace with the requirements of equilibrium so that the star will begin to contract.

(This is, in fact, indicated by the factor  $z^{1/8}$  in Eq. (55) for the stellar radius;  $z$  is proportional to the hydrogen concentration.) Gravitational attraction will then supply a large part of the energy. The contraction will continue until a new equilibrium is reached. For "light" stars of mass less than  $6\mu^{-2}$  sun masses (reference 1, p. 507), the electron gas in the star will become degenerate and a white dwarf will result. In the white dwarf state, the necessary energy production is extremely small so that such a star will have an almost unlimited life. This evolution was already suggested by Strömgren.<sup>1</sup>

For heavy stars, it seems that the contraction can only stop when a neutron core is formed. The difficulties encountered with such a core<sup>46</sup> may not be insuperable in our case because most of the hydrogen has already been transformed into heavier and more stable elements so that the energy evolution at the surface of the core will be by gravitation rather than by nuclear reactions. However, these questions obviously require much further investigation.

These investigations originated at the Fourth Washington Conference on Theoretical Physics, held in March, 1938 by the George Washington University and the Department of Terrestrial Magnetism. The author is indebted to Professors Strömgren and Chandrasekhar for information on the astrophysical data and literature, to Professors Teller and Gamow for discussions, and to Professor Konopinski for a critical revision of the manuscript.

<sup>46</sup> G. Gamow and E. Teller, Phys. Rev. 53, 929(A), 608(L) (1938).

## **Energy Production in Stars**

*Nobel Lecture (1967)*

This paper summarizes both the  $H + H$  reaction and the CN cycle. It compares the energy production by the two reaction chains. It also gives a brief history of the ideas of energy production, and discusses the evolution of stars after exhaustion of the hydrogen in the center of the star.

# ENERGY PRODUCTION IN STARS

by

H. A. BETHE

Cornell University

Nobel Lecture, December 11, 1967

## HISTORY

From time immemorial people must have been curious to know what keeps the sun shining. The first scientific attempt at an explanation was by Helmholtz about one hundred years ago, and was based on the force most familiar to physicists at the time, gravitation. When a gram of matter falls to the sun's surface it gets a potential energy

$$E_{\text{pot}} = -GM/R = -1.91 \cdot 10^{15} \text{ erg/gm} \quad (1)$$

where  $M = 1.99 \cdot 10^{33}$  gm is the sun's mass,  $R = 6.96 \cdot 10^{10}$  cm its radius, and  $G = 6.67 \cdot 10^{-8}$  the gravitational constant. A similar energy was set free when the sun was assembled from interstellar gas or dust in the dim past; actually somewhat more, because most of the sun's material is located closer to its center, and therefore has a numerically larger potential energy. One-half of the energy set free is transformed into kinetic energy according to the well-known virial theorem of mechanics. This will permit us later to estimate the temperature in the sun. The other half of the potential energy is radiated away. We know that at present the sun radiates

$$\epsilon = 1.96 \text{ erg/gm sec} \quad (2)$$

Therefore, if gravitation supplies the energy, there is enough energy available to supply the radiation for about  $10^{15}$  sec which is about 30 million years.

This was long enough for nineteenth century physicists, and certainly a great deal longer than man's recorded history. It was not long enough for the biologists of the time. Darwin's theory of evolution had just become popular, and biologists argued with Helmholtz that evolution would require a longer time than 30 million years, and that therefore his energy source for the sun was insufficient. They were right.

At the end of the 19th century, radioactivity was discovered by Becquerel and the two Curie's who received one of the first Nobel prizes for this discovery. Radioactivity permitted a determination of the age of the earth, and more recently, of meteorites which indicate the time at which matter in the solar system solidified. On the basis of such measurements the age of the sun is estimated to be 5 milliards of years, within about 10 %. So gravitation is not sufficient to supply its energy over the ages.

Eddington, in the 1920's, investigated very thoroughly the interior constitution of the sun and other stars, and was much concerned about the sources of stellar energy. His favorite hypothesis was the complete annihilation of

matter, changing nuclei and electrons into radiation. The energy which was to be set free by such a process, if it could occur, is given by the Einstein relation between mass and energy and is

$$c^2 = 9 \cdot 10^{20} \text{ erg/gm} \quad (3)$$

This would be enough to supply the sun's radiation for 1500 milliards of years. However nobody has ever observed the complete annihilation of matter. From experiments on earth we know that protons and electrons do not annihilate each other in  $10^{30}$  years. It is hard to believe that the situation would be different at a temperature of some 10 million degrees such as prevails in the stars, and Eddington appreciated this difficulty quite well.

From the early 1930's it was generally assumed that the stellar energy is produced by nuclear reactions. Already in 1929, Atkinson and Houtermans<sup>1</sup> concluded that at the high temperatures in the interior of a star, the nuclei in the star could penetrate into other nuclei and cause nuclear reactions, releasing energy. In 1933, particle accelerators began to operate in which such nuclear reactions were actually observed. They were found to obey very closely the theory of Gamow, Condon and Gurney, on the penetration of charged particles through potential barriers. In early 1938, Gamow and Teller<sup>2</sup> revised the theory of Atkinson and Houtermans on the rate of "thermonuclear" reactions, i.e. nuclear reactions occurring at high temperature. At the same time, Weizsäcker<sup>3</sup> speculated on the reactions which actually might take place in the stars.

In April 1938, Gamow assembled a small conference of physicists and astrophysicists in Washington, D.C. This conference was sponsored by the Department of Terrestrial Magnetism of the Carnegie Institution. At this Conference, the astrophysicists told us physicists what they knew about the internal constitution of the stars. This was quite a lot, and all their results had been derived without knowledge of the specific source of energy. The only assumption they made was that most of the energy was produced "near" the center of the star.

#### PROPERTY OF STARS

The most easily observable properties of a star are its total luminosity and its surface temperature. In relatively few cases of nearby stars, the mass of the star can also be determined.

Figure 1 shows the customary Hertzsprung-Russell diagram. The luminosity, expressed in terms of that of the sun, is plotted against the surface temperature, both on a logarithmic scale. Conspicuous is the main sequence, going from upper left to lower right, i.e. from hot and luminous stars to cool and faint ones. Most stars lie on this sequence. In the upper right are the Red Giants, cool but brilliant stars. In the lower left are the White Dwarfs, hot but faint. We shall be mainly concerned with the main sequence. After being assembled by gravitation, stars spend the most part of their life on the main sequence, then develop into red giants, and in the end, probably into white dwarfs. The figure shows that typical surface temperatures are of the order of  $10^4$  K.

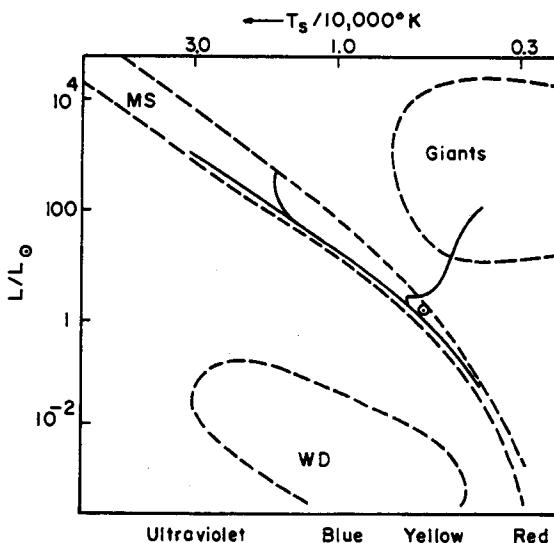


Fig. 1.  
Hertzsprung-Russell diagram.  
From E. E. Salpeter, in "Apollo and the Universe", Science Foundation for Physics, University of Sydney, Australia (1967).

Figure 2 gives the relation between mass and luminosity in the main sequence. At the upper end, beyond about 15 sun masses, the mass determinations are uncertain. It is clear, however, that luminosity increases rapidly with mass. For a factor of 10 in mass, the luminosity increases by a factor of about 3000, hence the energy production per gram is about 300 times larger.

To obtain information on the interior constitution of the stars, astrophysicists integrate two fundamental equations. Pioneers in this work have been Eddington, Chandrasekhar and Strömgren. The first equation is that of hydrostatic equilibrium

$$\frac{dP}{dr} = -G M(r) \frac{\rho(r)}{r^2} \quad (4)$$

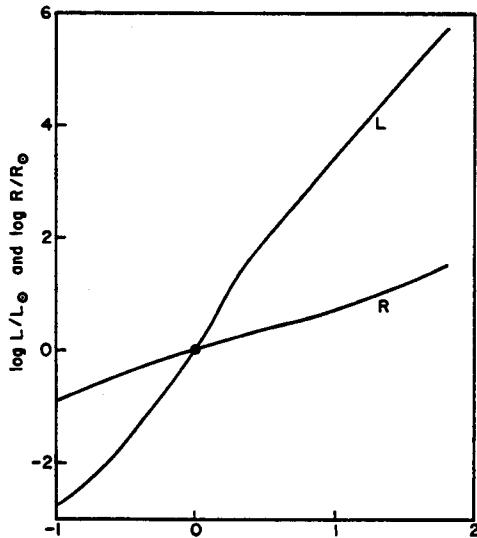


Fig. 2.  
Luminosity and radius of stars vs. mass. Abscissa is  $\log M/M_\odot$ . Data from C. W. Allen, *Astrophysical Quantities* (Athlone Press, 1963), p. 203. The curve for  $\log L/L_\odot$  holds for all stars, that for  $R/R_\odot$  only for the stars in the main sequence. The symbol  $\odot$  refers to the sun.

in which  $P$  is the pressure at distance  $r$  from the center,  $\rho$  is the density and  $M(r)$  is the total mass inside  $r$ . The second equation is that of radiation transport

$$\frac{1}{\kappa \rho} \frac{d}{dr} (\kappa a c T^4) = - \frac{L(r)}{4\pi r^2} \quad (5)$$

Here  $\kappa$  is the opacity of the stellar material for black-body radiation of the local temperature  $T$ ,  $a$  is the Stefan-Boltzmann constant, and  $L(r)$  is the flux of radiation at  $r$ . The value of  $L$  at the surface  $R$  of the star is the luminosity. In the stars we shall discuss, the gas obeys the equation of state

$$P = RT\rho/\mu \quad (6)$$

where  $R$  is the gas constant, while  $\mu$  is the mean molecular weight of the stellar material. If  $X$ ,  $Y$  and  $Z$  are respectively concentrations by mass of hydrogen, helium and all heavier elements, and if all gases are fully ionized, then

$$\mu^{-1} = 2X + \frac{3}{4}Y + \frac{1}{2}Z \quad (7)$$

In all stars except the very oldest ones, it is believed that  $Z$  is between 0.02 and 0.04; in the sun at present,  $X$  is about 0.65, hence  $Y=0.33$  and  $\mu=0.65$ . In many stars the chemical composition, especially  $X$  and  $Y$ , vary with position  $r$ . The opacity is a complicated function of  $Z$  and  $T$ , but in many cases it behaves like

$$\kappa = C \rho T^{-3.5} \quad (8)$$

where  $C$  is a constant.

The integration of (4) and (5) in general requires computers. However an estimate of the central temperature may be made from the virial theorem which we mentioned in the beginning. According to this, the average thermal energy per unit mass of the star is one-half of the average potential energy. This leads to the estimate of the thermal energy per particle at the center of the star,

$$k T_c = \alpha \mu G H M/R \quad (9)$$

in which  $H$  is the mass of the hydrogen atom, and  $\alpha$  is a constant whose magnitude depends on the specific model of the star but is usually about 1 for main sequence stars. Using this value, and (1), we find for the central temperature of the sun

$$T_{c6} = 14 \quad (10)$$

where  $T_6$  denotes the temperature in millions of degrees, here and in the following. A more careful integration of the equations of equilibrium by Demarque and Percy<sup>4</sup> gives

$$T_{c6} = 15.7; \rho_c = 158 \text{ gm/cm}^3 \quad (11)$$

Originally Eddington had assumed that the stars contain mainly heavy elements, from carbon on up. In this case  $\mu=2$  and the central temperature is increased by a factor of 3, to about 40 million degrees; this led to contradictions with the equation of radiation flow, (5), if the theoretical value of the opacity was used. Strömgren pointed out that these contradictions can be

resolved by assuming the star to consist mainly of hydrogen, which is also in agreement with stellar spectra. In modern calculations the three quantities X, Y, Z, indicating the chemical composition of the star, are taken to be parameters to be fixed so as to fit all equations of stellar equilibrium.

#### THERMONUCLEAR REACTIONS

All nuclei in a normal star are positively charged. In order for them to react they must penetrate each others Coulomb potential barrier. The wave mechanical theory of this shows that in the absence of resonances, the cross section has the form

$$\sigma(E) = \frac{S(E)}{E} \exp\left(-\sqrt{\frac{E_G}{E}}\right) \quad (12)$$

where E is the energy of the relative motion of the two colliding particles, S (E) is a coefficient characteristic of the nuclear reaction involved and

$$E_G = 2M(\pi Z_0 Z_1 e^2/h)^2 = (2\pi Z_0 Z_1)^2 E_{Bohr} \quad (13)$$

Here M is the reduced mass of the two particles, Z<sub>0</sub> and Z<sub>1</sub> their charges, and E<sub>Bohr</sub> is the Bohr energy for mass M and charge 1. (13) can be evaluated to give

$$E_G = .979 W \text{ Mev} \quad (14)$$

with

$$W = A Z_0^2 Z_1^2 \quad (14 \text{ a})$$

$$A = A_0 A_1 / (A_0 + A_1) \quad (14 \text{ b})$$

in which A<sub>0</sub>, A<sub>1</sub> are the atomic weights of the two colliding particles. For most nuclear reactions S (E) is between 10 Mev-barns and 1 kev-barn.

The gas at a given r in the star has a given temperature so that the particles have a Boltzmann energy distribution. The rate of nuclear reactions is then proportional to

$$(8/\pi M)^{1/2} (k T)^{-3/2} \int \sigma(E) E \exp(-E/kT) dE \quad (15)$$

It is most convenient<sup>5</sup> to write for the rate of disappearance of one of the reactants

$$dX_0/dt = -[01] X_0 X_1 \quad (16)$$

where X<sub>0</sub> and X<sub>1</sub> are the concentrations of the reactants by mass, and

$$[01] = 7.8 \cdot 10^{11} (Z_0 Z_1 / A)^{1/3} S_{eff} \rho T_6^{-2/3} e^{-\tau} \quad (17)$$

$$\tau = 42.487 (W/T_6)^{1/3} \quad (17 \text{ a})$$

Since the reaction cross section (12) increases rapidly with energy, the main contribution to the reaction comes from particles which have an energy many times the average thermal energy. Indeed the most important energy is

$$E_0 = (\tau/3) k T \quad (18)$$

For T=13 which is an average for the interior of the sun, we have

$\tau/3 = 4.7$  for the reaction H+H



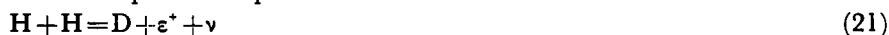
It is also easy to see from (17) that the temperature dependence of the reaction rate is

$$\frac{d \ln [01]}{d \ln T} = \frac{\tau - 2}{3} \quad (20)$$

### NUCLEAR REACTIONS IN MAIN SEQUENCE STARS

Evidently, at a given temperature and under otherwise equal conditions, the reactions which can occur most easily are those which have the smallest possible value of  $W$ , (14 a). This means that at least one of the interacting nuclei should be a proton,  $A_0 = Z_0 = 1$ . Thus we may examine the reactions involving protons.

The simplest of all possible reactions is



( $e^+$  = positron,  $\nu$  = neutrino).

This was first suggested by Weizsäcker<sup>3</sup>, and calculated by Critchfield and Bethe<sup>4</sup>. The reaction is of course exceedingly slow because it involves the beta disintegration. Indeed the characteristic factor  $S$  is

$$S(E) = 3.36 \cdot 10^{-25} \text{ Mev-barns} \quad (22)$$

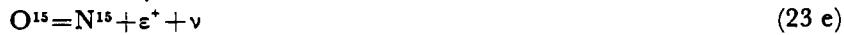
This has been derived on purely theoretical grounds, using the known coupling constant of beta disintegration; the value is believed to be accurate to 5 % or better. There is no chance of observing such a slow reaction on earth, but in the stars we have almost unlimited time, and a large supply of protons of high energy. As we shall see presently, the rate of energy production by this simple reaction fits the observed energy production in the sun very well.

The deuterons formed in (21) will quickly react further, and the end product is  $He^4$ . We shall discuss the reactions in more detail later on.

The proton-proton reaction (21), although it predicts the correct energy production in the sun, has a rather weak dependence on temperature. According to (19), (20), it behaves about as  $T^4$ . Since central temperatures change only little from the sun to more massive stars, the energy production by this reaction does likewise. However as we have seen in Fig. 2, the observed energy production increases dramatically with increasing mass. Therefore there must exist nuclear reactions which are more strongly dependent on temperature; these must involve heavier nuclei.

Stimulated by the Washington Conference of April 1938, and following the argument just mentioned, I examined<sup>7</sup> the reactions between protons and other nuclei, going up in the periodic system. Reactions between  $H$  and  $He^4$  lead nowhere, there being no stable nucleus of mass 5. Reactions of  $H$  with  $Li$ ,  $Be$  and  $B$ , as well as with deuterons, are all very fast at the central temperature of the sun, but just this speed of the reaction rules them out: the partner of  $H$  is very quickly used up in the process. In fact, and just because of this reason, all the elements mentioned, from deuterium to boron, are extremely rare on earth and in the stars, and can therefore not be important sources of energy.

The next element, carbon, behaves quite differently. In the first place, it is an abundant element, probably making up about 1 % by mass of any newly formed star. Secondly, in a gas of stellar temperature, it undergoes a cycle of reactions, as follows



Reactions a, c, and d are radiative captures; the proton is captured by the nucleus and the energy emitted in the form of gamma rays; these are then quickly converted into thermal energy of the gas. For reactions of this type,  $S(E)$  is of the order of 1 kev-barn. Reactions b and e are simply spontaneous beta decays, with lifetimes of 10 and 2 minutes respectively, negligible in comparison with stellar times. Reaction f is the most common type of nuclear reaction, with 2 nuclei resulting from the collision;  $S(E)$  for such reactions is commonly of the order of Mev-barns.

Reaction f is in a way the most interesting because it closes the cycle: we reproduce the  $\text{C}^{12}$  which we started from. In other words, carbon is only used as a catalyst; the result of the reaction is a combination of 4 protons and 2 electrons<sup>7</sup> to form one  $\text{He}^4$  nucleus. In this process two neutrinos are emitted, taking away about 2 Mev energy together. The rest of the energy, about 25 Mev per cycle, is released usefully to keep the sun warm.

Making reasonable assumptions of the reaction strength  $S(E)$ , on the basis of general nuclear physics, I found in 1938 that the carbon-nitrogen cycle gives about the correct energy production in the sun. Since it involves nuclei of relatively high charge, it has a strong temperature dependence, as given in (19). The reaction with  $\text{N}^{14}$  is the slowest of the cycle and therefore determines the rate of energy production; it goes about as  $T^{24}$  near solar temperature. This is amply sufficient to explain the high rate of energy production in massive stars<sup>8</sup>.

#### EXPERIMENTAL RESULTS

To put the theory on a firm basis, it is important to determine the strength factor  $S(E)$  for each reaction by experiment. This has been done under the leadership of W. A. Fowler<sup>10</sup> of the California Institute of Technology in a monumental series of papers extending over a quarter of a century. Not only have all the reactions in (23) been observed, but in all cases  $S(E)$  has been accurately determined.

The main difficulty in this work is due to the resonances which commonly occur in nuclear reactions. Fig. 3 shows the cross section of the first reaction<sup>9</sup> (23 a), as a function of energy. The measured cross sections extend over a factor of  $10^7$  in magnitude; the smallest ones are  $10^{-11}$  barns =  $10^{-35}$  cm<sup>2</sup> and therefore clearly very difficult to observe. The curve shows a resonance at

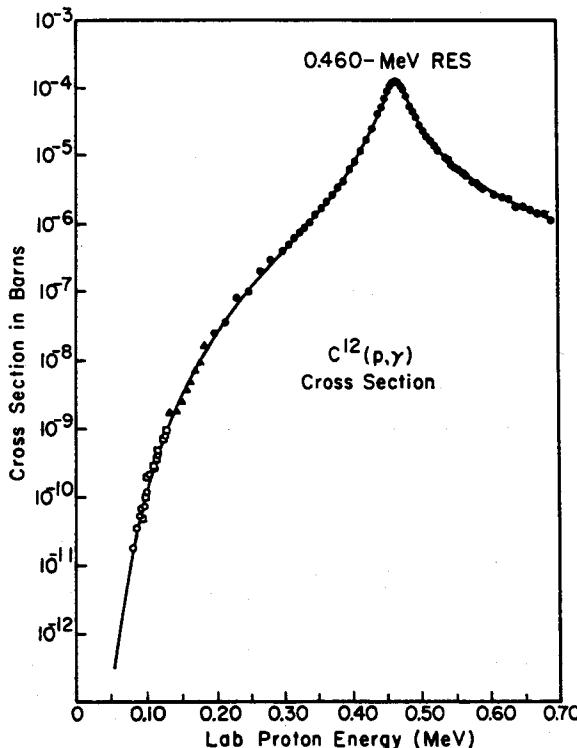


Fig. 3.  
Cross section for the reaction  $C^{12}(p,\gamma)$ , as a function of the proton energy. From Fowler, Caughlan and Zimmerman, reference 5.

460 kev. The solid curve is determined from nuclear reaction theory, on the basis of the existence of that resonance. The fit of the observed points to the calculated curve is impressive. Similar results have been obtained on the other three proton-capture reactions in (23).

On the basis of Fig. 3 we can confidently extrapolate the measurements to lower energy. As we mentioned in (18), the most important energy contributing to the reaction rate is about  $20 \text{ kT}$ . For  $T_e = 13$ , we have  $kT = 1.1 \text{ kev}$ ; so we are most interested in the cross section around 20 kev. This is much too low an energy to observe the cross section in the laboratory; even at 100 kev, the cross section is barely observable. So quite a long extrapolation is required. This can be done with confidence provided there are no resonances close to  $E=0$ . Therefore a great deal of experimental work has gone into the search for such resonances.

The resonances exist of course in the compound nucleus, i.e. the nucleus obtained by adding the two initial reactants. To find resonances near the threshold of the reactions (23), it is necessary to produce the same compound nucleus from other initial nuclei, e.g., in the reaction between  $N^{14}$  and H, the compound nucleus  $O^{15}$  is formed. To investigate its levels Hensley<sup>11</sup> at CalTech studied the reaction



He found indeed a resonance 20 kev below the threshold for  $N^{14} + H$  which in principle might enhance the process (23 d). However the state in  $O^{15}$  was

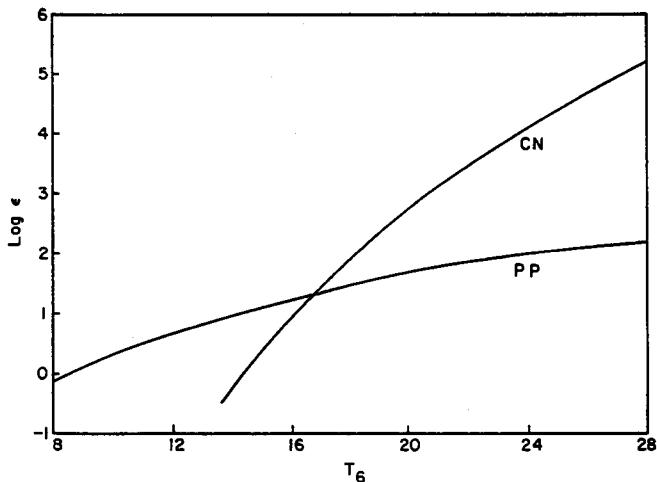


Fig. 4.

The energy production, in erg/gm sec, as a function of the temperature in millions of degrees. For the proton-proton reaction (P P) and the carbon-nitrogen cycle (C N). Concentrations assumed X=Y=0.5, Z=0.02. Calculated from Table 8 and 9 of Reeves, reference 12.

found to have a spin  $J=7/2$ . Therefore, even though  $N^{14}$  has  $J=1$  and the proton has a spin of  $1/2$ , we need at least an orbital momentum  $\lambda=2$ , to reach this resonant state in  $O^{15}$ . The cross section for such a high orbital momentum is reduced by at least a factor  $10^4$ , compared to  $\lambda=0$ , so that the near-resonance does not in fact enhance the cross section  $N^{14}+H$  appreciably. This cross section can then be calculated by theoretical extrapolation from the measured range of proton energies, and the same is true for the other reactions in the cycle (23).

On this basis, Fowler and others have calculated the rate of reactions in the C N cycle. A convenient tabulation has been given by Reeves<sup>12</sup>; his results are plotted in Fig. 4. This figure gives the energy production per gram per second as a function of temperature. We have assumed X=0.5, Z=0.02. The figure shows that at low temperature the H+H reaction dominates, at high temperatures the C+N cycle; the crossing point is at  $T_6=13$ ; here the energy production is 7 erg/gm sec. The average over the entire sun is obviously smaller, and the result is compatible with an average production of 2 erg/gm sec.

The energy production in the main sequence can thus be considered as well understood.

An additional point should be mentioned. Especially at higher temperature, when the C N cycle prevails, there is also a substantial probability for the reaction chain



This chain is not cyclic but feeds into the C N cycle. It is customary to speak of the whole set of reactions as the C N O bi-cycle. The effect of reactions

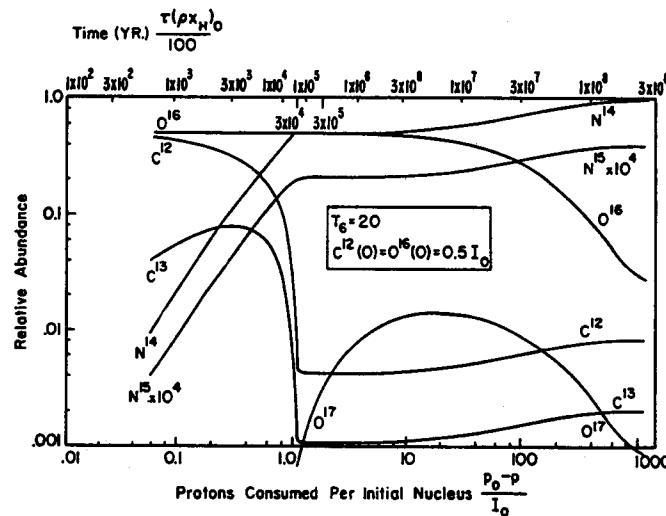


Fig. 5.

Variation with time of the abundances of various elements involved in the C N O cycle. It is assumed that initially C<sup>12</sup> and O<sup>16</sup> have the same abundance while that of N<sup>14</sup> is small. From G. R. Caughlan, Astroph. J. (1967).

(25) is that O<sup>16</sup> initially present will also contribute to the reactants available, and thus increase the reaction rate of the C N cycle somewhat. This has been taken into account in Fig. 4.

If equilibrium is established in the C N O bi-cycle, eventually most of the nuclei involved will end up as N<sup>14</sup> because this nucleus has by far the longest lifetime against nuclear reactions. There is no observable evidence for this; in fact wherever the abundance can be observed, C and O tend to be at least as abundant as N. However this is probably due to the fact that the interior of a star stays well separated from its surface; there is very little mixing. Astrophysicists have investigated the circumstances when mixing is to be expected, and have found that surface abundances are quite compatible with these expectations. In the interstellar material which is used to form stars, we have reason to believe that C and O are abundant and N is rare. This will be discussed later.

#### THE COMPLETION OF THE PROTON-PROTON CHAIN

The initial reaction (21) is followed almost immediately by



The fate of He<sup>3</sup> depends on the temperature. Below about T<sub>e</sub>=15, the He<sup>3</sup> builds up sufficiently so that two such nuclei react with each other according to

(27)

This reaction has an unusually high S (E)=5 Mev-barns<sup>5</sup>. At higher temperature, the reaction



competes favorably with (27). The  $\text{Be}^7$  thus formed may again react in one of two ways



At about  $T_e = 20$ , reaction (29 b) begins to dominate over (29 a). (29 b) is followed by (29 c) which emits neutrinos of very high energy. Davis<sup>13</sup>, at Brookhaven, is attempting to observe these neutrinos.

#### EVOLUTION OF A STAR

A main sequence star uses up its hydrogen preferentially near its center where nuclear reactions proceed most rapidly. After a while, the center has lost almost all its hydrogen. For stars of about twice the luminosity of the sun, this happens in less than  $10^{14}$  years which is approximately the age of the universe, and also the age of stars in the globular clusters. We shall now discuss what happens to a star after it has used up the hydrogen at the center. Of course, in the outside regions hydrogen is still abundant.

This evolution of a star was first calculated by Schwarzschild<sup>14</sup> who has been followed by many others; we shall use recent calculations by Iben<sup>15</sup>. When hydrogen gets depleted, not enough energy is produced near the center to sustain the pressure of the outside layers of the star. Hence gravitation will cause the center to collapse. Thereby, higher temperatures and densities are achieved. The temperature also increases farther out where there is still hydrogen left, and this region now begins to burn. After a relatively short time, a shell of H, away from the center, produces most of the energy; this shell gradually moves outward and gets progressively thinner as time goes on.

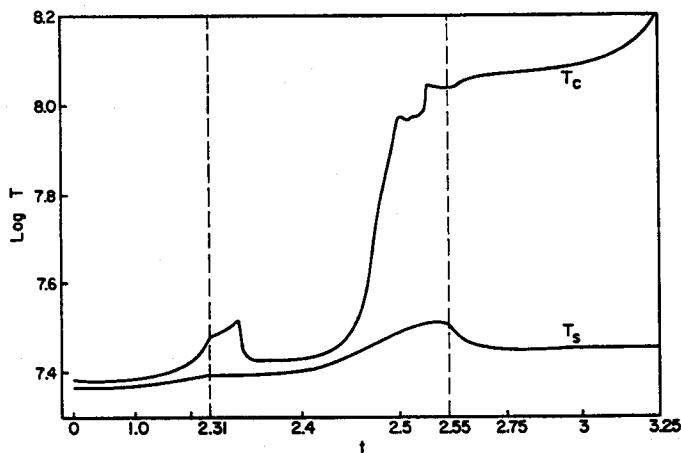


Fig. 6.

Evolution of a star of 3 solar masses, according to I. Iben, *Astroph. J.* 142, 1447 (1965). Abscissa is time in units of  $10^8$  years (note the breaks in scale at  $t=2.31$  and  $2.55$ ). I. Temperature (on logarithmic scale):  $T_c$ =temperature at center of star,  $T_s$ =same at mid-point of source of energy generation, which, after  $t=2.48$  is a thin shell.  $T_c$  increases enormously,  $T_s$  stays almost constant.

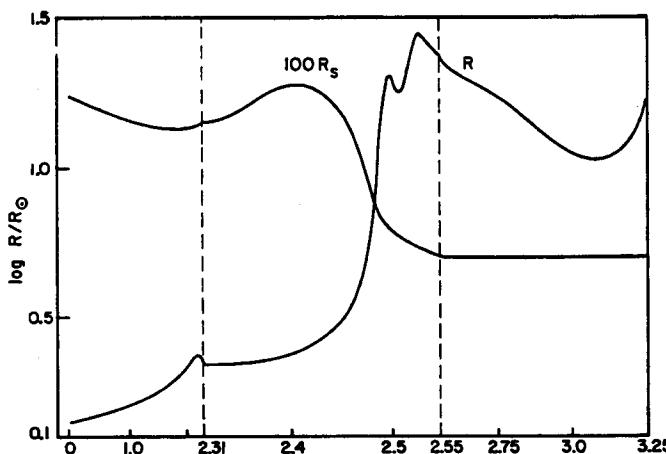


Fig. 7.

Evolution of a star, see caption to Fig. 6. II. Radius, in units of that of the sun, on logarithmic scale.  $R$  = total radius,  $100 R_s = 100$  times the radius of mid-point of energy source.  $R$  increases tremendously, while  $R_s$  shrinks somewhat.

At the same time, the region of the star outside the burning shell expands. This result follows clearly from all the many numerical computations on this subject. The physical reason is not clear. One hypothesis is that it is due to the discontinuity in mean molecular weight: Inside the shell, there is mostly helium, of  $\mu=4/3$ , outside we have mostly hydrogen, and  $\mu=0.65$ . Another suggestion is that the flow of radiation is made difficult by the small radius of the energy source, and that this has to be compensated by lower density just outside the source.

By this expansion the star develops into a red giant. Indeed, in globular clusters (which, as I mentioned, are made up of very old stars), all the more luminous stars are red giants. In the outer portion of these stars, radiative transport is no longer sufficient to carry the energy flow; therefore convection of material sets in in these outer regions. This convection can occupy as much as the outer 80 % of the mass of the star; it leads to intimate mixing of the material in the convection zone.

Iben<sup>15</sup> has discussed a nice observational confirmation of this convectional mixing. The star Capella is a double star, each component having a mass of about 3 solar masses, and each being a red giant. The somewhat lighter star, "Capella F" (its spectral type is F) shows noticeable amounts of Li in its spectrum, while the somewhat heavier Capella G shows at least 100 times less Li. It should be expected that G, being heavier, is farther advanced in its evolution. Iben now gives arguments that the deep-reaching convection and mixing which we just discussed, will occur just between the evolution phases F and G. By convection, material from the interior of the star will be carried to the surface; this material has been very hot and has therefore burned up its Li. Before deep convection sets in (in star F) the surface Li never sees high temperatures and thus is preserved.

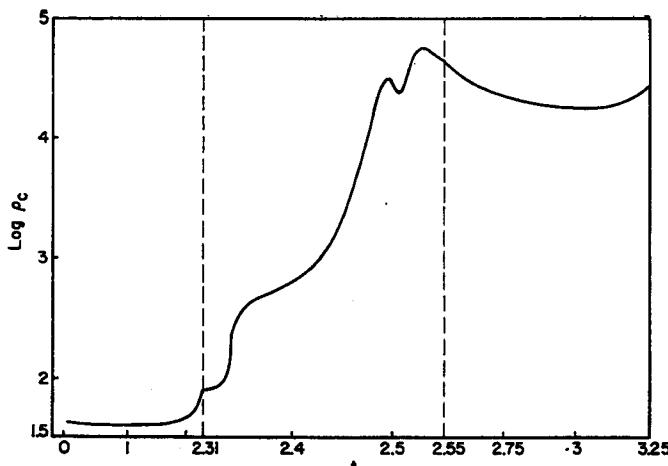


Fig. 8.

Evolution of a star, see caption to Fig. 6. III. Density, on logarithmic scale, at the center of the star. This quantity increases about 1000-fold.

Following the calculations of Iben we have plotted in Figures 6 to 9 the development of various important quantities in the history of a star of mass = 3 solar masses. The time is in units of  $10^8$  years. Since the developments go at very variable speed, the time scale has been broken twice, at  $t=2.31$  and  $t=2.55$ . In between is the period during which the shell source develops.

During this period the central temperature rises spectacularly (Fig. 6), from about  $T_e=25$  to  $T_e=100$ . At the same time the radius increases from about 2 to 30 solar radii; subsequently, it decreases again to about 15 (Fig. 7). The central density, starting at about 40, increases in the same period to about  $5 \cdot 10^4$ . The luminosity (Fig. 9) does not change spectacularly, staying always between 100 and 300 times that of the sun.

While the inside and the outside of the star undergo such spectacular changes, the shell in which the hydrogen is actually burning, does not change very much. Fig. 9 shows  $m$ , the fraction of the mass of the star enclosed by the burning shell. Even at the end of the calculation,  $t=3.25$ , this is only  $m=.2$ . This means that only 20 % of the hydrogen in the star has burned after all this development. Fig. 6, curve  $T_s$ , shows the temperature in the burning shell which stays near 25 million degrees all the time. Fig. 7, curve  $R_s$ , shows the radius of the shell, in units of the solar radius; during the critical time when the shell is formed this radius drops from about .15 to .07. This is of course the mechanism by which the shell is kept at the temperature which originally prevailed at the center.

In the meantime, the temperature at the center increases steadily. When it reaches about  $T_e=100$ , the  $\text{He}^4$  which is abundant at the center, can undergo nuclear reactions. The first of these, which occurs at the lowest temperature (about  $T_e=90$ ) is



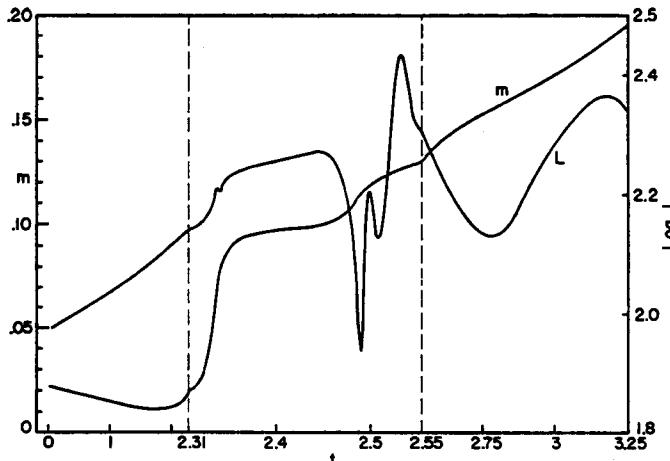


Fig. 9.

Evolution of a star, see caption to Fig. 6. IV. Curve L, luminosity relative to that of the sun, on logarithmic scale. This quantity does not change very much during the life of the star. Curve m, fraction of the mass of the star enclosed by energy-producing shell, on linear scale. This fraction increases slowly with time.

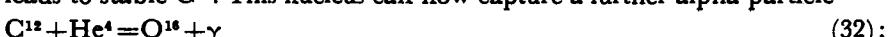
While this reaction goes on, the central temperature remains fairly constant. However, there is not much  $N^{14}$  so the reaction soon stops (after about  $0.02 \cdot 10^8$  years), and the center contracts further.

The next reaction makes use entirely of the abundant  $He^4$ , viz.



This reaction has the handicap of requiring a simultaneous collision of 3 alpha particles. This would be extremely unlikely were it not for the fact that it is favored by a *double* resonance. Two alpha particles have nearly the same energy as the unstable nucleus  $Be^8$ , and further  $Be^8 + He^4$  has almost the same energy as an excited state of  $C^{12}$ . This reaction can of course not be observed in the laboratory but the two contributing resonances can be. The importance of the first resonance was first suggested by Salpeter<sup>16</sup>, the second by Hoyle<sup>17</sup>. Recent data indicate that (31) requires a temperature of about  $T_e = 110$ , at the central densities corresponding to  $t = 2.5$ , i.e.  $\rho_c > 10^4$ . Once this reaction sets in, the central temperature does not rise very fast any more.

Reaction (31) is most important for the buildup of elements. Early investigators<sup>3,7</sup> had great trouble with bridging the gap between  $He^4$  and  $C^{12}$ . Two nuclei in this gap, mass 5 and mass 8, are completely unstable, the rest disintegrate in a very short time under stellar conditions. Reaction (31) however leads to stable  $C^{12}$ . This nucleus can now capture a further alpha particle



the temperatures required for this are about the same as for (31). There is also some capture of alpha particles by  $O^{16}$  leading to  $Ne^{20}$ , but the next step,  $Ne^{20} \rightarrow Mg^{24}$ , cannot occur appreciably at these temperatures; instead, the helium gets used up in forming  $C^{12}$ ,  $O^{16}$  and some  $Ne^{20}$ .

Helium is depleted first in the center, and now the same process repeats which previously took place with hydrogen. A shell of burning He is formed, at a smaller radius than the H shell, and of course at a higher temperature. The center of the star now contracts further by gravitation and reaches still higher temperatures.

#### BUILDUP AND DISPERSAL OF ELEMENTS

The further developments of a massive star are more speculative. However the theory of Hoyle and collaborators<sup>18</sup> is likely to be correct.

The center of the star heats up until the newly formed carbon nuclei can react with each other. This happens at a temperature of roughly  $10^9$  degrees. Nuclei like  $Mg^{24}$  or  $Si^{28}$  can be formed. There are also more complicated mechanisms in which we first have a capture reaction with emission of a gamma ray, followed by capture of this gamma ray in another nucleus which releases  $He^4$ . This  $He^4$  can then enter further nuclei and build up the entire chain of stable nuclei up to the most stable Fe. Not much energy is released in all of these processes.

The center of the star contracts further and gets still hotter. At very high temperatures, several milliards of degrees, thermal equilibrium is no longer strongly in favor of nuclei of the greatest binding energy. Instead, endothermic processes can take place which destroy some of the stable nuclei already formed. In the process, alpha particles, protons and even neutrons may be released. This permits the buildup of elements beyond Fe, up to the top of the periodic table. Because of the high temperatures involved all this probably goes fairly fast, perhaps in thousands of years.

During this stage, nuclear processes tend to consume rather than release energy. Therefore they no longer oppose the gravitational contraction so that contraction continues unchecked. It is believed that this will lead to an unstable situation. Just as the first contraction, at the formation of the H shell source, led to an expansion of the outer envelope of the star, a similar outward expansion is expected now. But time scales are now short, and this expansion may easily be an explosion. Hoyle, et al., have suggested this as the mechanism for a supernova.

In a supernova explosion much of the material of the star is ejected into interstellar space. We see this, e.g., in the Crab Nebula. The ejected material probably contains the heavy elements which have been formed in the interior of the massive star. Thus heavy elements get into the interstellar gas, and can then be collected again by newly forming stars. It is believed that this is the way how stars get their heavy elements. This means that most of the stars we see, including our sun, are at least second generation stars, which have collected the debris of earlier stars which have suffered a supernova explosion.

To clinch this argument it must be shown that heavy elements cannot be produced in other ways. This has indeed been shown by Fowler<sup>19</sup>. He has investigated the behavior of the enormous gas cloud involved in the original "Big Bang", and its development with time. He has shown that temperatures and densities, as functions of time, are such that heavy elements beginning

with C cannot be produced. The only element which can be produced in the big bang is He<sup>4</sup>.

If all this is true, stars have a life cycle much like animals. They get born, they grow, they go through a definite internal development, and finally they die, to give back the material of which they are made so that new stars may live.

I am very grateful to Professor E. E. Salpeter for his extensive help in preparing this paper.

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## The Electromagnetic Shift of Energy Levels

*Phys. Rev.* **72** (4), 339–341 (1947)

Lamb and Rutherford had observed that the 2s level of the H atom lies slightly above the  $2p_{1/2}$  level whereas, in Dirac theory, the two levels should coincide. This was announced at the Shelter Island Conference on theoretical physics in June 1947. At that conference also, the interaction of the electron with its own electromagnetic field was discussed which, by straightforward quantum electrodynamics, was infinite. H. Kramers suggested that for a free electron, this interaction is already included in the observed mass of the electron, and so only the difference between a bound and a free electron should be observable. This is the basis of the present paper.

The agreement of the result, 1040 MHz, with observation encouraged Schwinger and Feynman to develop two independent relativistic theories of renormalization. Dyson proved that they are equivalent.

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## The Electromagnetic Shift of Energy Levels

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BY very beautiful experiments, Lamb and Rutherford<sup>1</sup> have shown that the fine structure of the second quantum state of hydrogen does not agree with the prediction of the Dirac theory. The 2s level, which according to Dirac's theory should coincide with the 2p<sub>1</sub> level, is actually higher than the latter by an amount of about 0.033 cm<sup>-1</sup> or 1000 megacycles. This discrepancy had long been suspected from spectroscopic measurements.<sup>2,3</sup> However, so far no satisfactory theoretical explanation has been given. Kemble and Present, and Pasternack<sup>4</sup> have shown that the shift of the 2s level cannot be

explained by a nuclear interaction of reasonable magnitude, and Uehling<sup>5</sup> has investigated the effect of the "polarization of the vacuum" in the Dirac hole theory, and has found that this effect also is much too small and has, in addition, the wrong sign.

Schwinger and Weisskopf, and Oppenheimer have suggested that a possible explanation might be the shift of energy levels by the interaction of the electron with the radiation field. This shift comes out infinite in all existing theories, and has therefore always been ignored. However, it is possible to identify the most strongly (linearly) divergent term in the level shift with an electromagnetic mass effect which must exist for a bound as well as for a free electron. This effect should

<sup>1</sup> Phys. Rev. 72, 241 (1947).

<sup>2</sup> W. V. Houston, Phys. Rev. 51, 446 (1937).

<sup>3</sup> R. C. Williams, Phys. Rev. 54, 558 (1938).

<sup>4</sup> E. C. Kemble and R. D. Present, Phys. Rev. 44, 1031 (1932); S. Pasternack, Phys. Rev. 54, 1113 (1938).

<sup>5</sup> E. A. Uehling, Phys. Rev. 48, 55 (1935).

properly be regarded as already included in the observed mass of the electron, and we must therefore subtract from the theoretical expression, the corresponding expression for a free electron of the same average kinetic energy. The result then diverges only logarithmically (instead of linearly) in non-relativistic theory: Accordingly, it may be expected that in the hole theory, in which the *main* term (self-energy of the electron) diverges only logarithmically, the result will be *convergent* after subtraction of the free electron expression.<sup>6</sup> This would set an effective upper limit of the order of  $mc^2$  to the frequencies of light which effectively contribute to the shift of the level of a bound electron. I have not carried out the relativistic calculations, but I shall assume that such an effective relativistic limit exists.

The ordinary radiation theory gives the following result for the self-energy of an electron in a quantum state  $m$ , due to its interaction with transverse electromagnetic waves:

$$W = -(2e^2/3\pi\hbar c^3)$$

$$\times \int_0^K k dk \sum_n |\mathbf{v}_{mn}|^2 / (E_n - E_m + k), \quad (1)$$

where  $k = \hbar\omega$  is the energy of the quantum and  $\mathbf{v}$  is the velocity of the electron which, in non-relativistic theory, is given by

$$\mathbf{v} = \mathbf{p}/m = (\hbar/im)\nabla. \quad (2)$$

Relativistically,  $\mathbf{v}$  should be replaced by  $c\alpha$  where  $\alpha$  is the Dirac operator. Retardation has been neglected and can actually be shown to make no substantial difference. The sum in (1) goes over all atomic states  $n$ , the integral over all quantum energies  $k$  up to some maximum  $K$  to be discussed later.

For a free electron,  $\mathbf{v}$  has only diagonal elements and (1) is replaced by

$$W_0 = -(2e^2/3\pi\hbar c^3) \int k dk v^2/k. \quad (3)$$

This expression represents the change of the kinetic energy of the electron for fixed mo-

mentum, due to the fact that electromagnetic mass is added to the mass of the electron. This electromagnetic mass is already contained in the experimental electron mass; the contribution (3) to the energy should therefore be disregarded. For a bound electron,  $v^2$  should be replaced by its expectation value,  $(\mathbf{v}^2)_{mn}$ . But the matrix elements of  $\mathbf{v}$  satisfy the sum rule

$$\sum_n |\mathbf{v}_{mn}|^2 = (\mathbf{v}^2)_{mm}. \quad (4)$$

Therefore the relevant part of the self-energy becomes

$$W' = W - W_0 = + \frac{2e^2}{3\pi\hbar c^3} \times \int_0^K dk \sum_n \frac{|\mathbf{v}_{mn}|^2 (E_n - E_m)}{E_n - E_m + k}. \quad (5)$$

This we shall consider as a true shift of the levels due to radiation interaction.

It is convenient to integrate (5) first over  $k$ . Assuming  $K$  to be large compared with all energy differences  $E_n - E_m$  in the atom,

$$W'' = \frac{2e^2}{3\pi\hbar c^3} \sum_n |\mathbf{v}_{mn}|^2 (E_n - E_m) \ln \frac{K}{|E_n - E_m|}. \quad (6)$$

(If  $E_n - E_m$  is negative, it is easily seen that the principal value of the integral must be taken, as was done in (6).) Since we expect that relativity theory will provide a natural cut-off for the frequency  $k$ , we shall assume that in (6)

$$K \approx mc^2. \quad (7)$$

(This does not imply the same limit in Eqs. (2) and (3).) The argument in the logarithm in (6) is therefore very large; accordingly, it seems permissible to consider the logarithm as constant (independent of  $n$ ) in first approximation.

We therefore should calculate

$$A = \sum_n A_{nm} = \sum_n |\mathbf{p}_{nm}|^2 (E_n - E_m). \quad (8)$$

This sum is well known; it is

$$\begin{aligned} A &= \sum_n |\mathbf{p}_{nm}|^2 (E_n - E_m) \\ &= -\hbar^2 \int \psi_m^* \nabla V \cdot \nabla \psi_m d\tau \\ &= \frac{1}{2} \hbar^2 \int \nabla^2 V \psi_m^2 d\tau = 2\pi\hbar^2 e^2 Z \psi_m^2(0). \end{aligned} \quad (9)$$

<sup>6</sup> It was first suggested by Schwinger and Weisskopf that hole theory must be used to obtain convergence in this problem.

for a nuclear charge  $Z$ . For any electron with angular momentum  $l \neq 0$ , the wave function vanishes at the nucleus; therefore, the sum  $A = 0$ . For example, for the  $2p$  level the negative contribution  $A_{1s,2p}$  balances the positive contributions from all other transitions. For a state with  $l = 0$ , however,

$$\psi_m^2(0) = (Z/na)^3/\pi, \quad (10)$$

where  $n$  is the principal quantum number and  $a$  is the Bohr radius.

Inserting (10) and (9) into (6) and using relations between atomic constants, we get for an  $S$  state

$$W_{ns}' = \frac{8}{3\pi} \left(\frac{e^2}{hc}\right)^3 \frac{Z^4}{n^3} \frac{K}{\langle E_n - E_m \rangle_m}, \quad (11)$$

where Ry is the ionization energy of the ground state of hydrogen. The shift for the  $2p$  state is negligible; the logarithm in (11) is replaced by a value of about  $-0.04$ . The average excitation energy  $\langle E_n - E_m \rangle_m$  for the  $2s$  state of hydrogen has been calculated numerically<sup>7</sup> and found to be 17.8 Ry, an amazingly high value. Using this figure and  $K = mc^2$ , the logarithm has the value 7.63, and we find

$$W_{ns}' = 136 \ln[K/(E_n - E_m)] \\ = 1040 \text{ megacycles.} \quad (12)$$

<sup>7</sup> I am indebted to Dr. Stehn and Miss Steward for the numerical calculations.

This is in excellent agreement with the observed value of 1000 megacycles.

A relativistic calculation to establish the limit  $K$  is in progress. Even without exact knowledge of  $K$ , however, the agreement is sufficiently good to give confidence in the basic theory. This shows

(1) that the level shift due to interaction with radiation is a real effect and is of finite magnitude,

(2) that the effect of the infinite electromagnetic mass of a point electron can be eliminated by proper identification of terms in the Dirac radiation theory,

(3) that an accurate experimental and theoretical investigation of the level shift may establish relativistic effects (e.g., Dirac hole theory). These effects will be of the order of unity in comparison with the logarithm in Eq. (11).

If the present theory is correct, the level shift should increase roughly as  $Z^4$  but not quite so rapidly, because of the variation of  $\langle E_n - E_m \rangle_m$  in the logarithm. For example, for  $\text{He}^+$ , the shift of the  $2s$  level should be about 13 times its value for hydrogen, giving  $0.43 \text{ cm}^{-1}$ , and that of the  $3s$  level about  $0.13 \text{ cm}^{-1}$ . For the x-ray levels  $LI$  and  $LII$ , this effect should be superposed upon the effect of screening which it partly compensates. An accurate theoretical calculation of the screening is being undertaken to establish this point.

This paper grew out of extensive discussions at the Theoretical Physics Conference on Shelter Island, June 2 to 4, 1947. The author wishes to express his appreciation to the National Academy of Science which sponsored this stimulating conference.

**Theory of the Effective Range in Nuclear Scattering**  
*Phys. Rev.* **76** (1), 38–50 (1949)

The scattering of neutrons or protons by protons, up to about 10 MeV, can be described by two parameters, the scattering length at zero energy and the effective range. The shape of the potential does not matter in this energy region. The theory is similar to an earlier one by Schwinger, but it is simpler. The two parameters are evaluated for the various scattering processes.

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## Theory of the Effective Range in Nuclear Scattering

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The scattering of neutrons up to about 10 or 20 Mev by protons can be described by two parameters, the scattering length at zero energy,  $a$ , and the effective range,  $r_0$ . A formula (16), expressing the phase shift in terms of  $a$  and  $r_0$  is derived; it is identical with one previously derived by Schwinger but the derivation is very much simpler. Reasons are given why the deviations from the simple formula are very small, as shown by the explicit calculations by Blatt and Jackson.

The theory is then applied to proton-proton scattering, with a similarly simple result. Moreover, a method is developed to compare proton-proton and proton-neutron scattering without explicit calculation of a nuclear potential.

The most recent experimental results are evaluated on the basis of the theory, and accurate values for the effective ranges are obtained for the triplet scattering of neutrons, and for proton-proton scattering. The nuclear force between two protons is found to differ by a slight amount, but beyond doubt, from that between neutron and proton in the singlet state. All actual results agree with those obtained by Breit and collaborators, and by Blatt and Jackson.

### I. INTRODUCTION

SCHWINGER<sup>1</sup> has shown that the phase shift  $\delta$  in the triplet neutron-proton scattering is related to the wave number  $k$  by the relation

$$k \cot \delta = -\gamma + \frac{1}{2}(\gamma^2 + k^2)r_0 + O(k^4r_0^3), \quad (1)$$

where  $\gamma$  is related to the deuteron binding energy,  $\epsilon$ , by

$$\epsilon = (\hbar^2/M)\gamma^2, \quad (2)$$

and  $r_0$  is a constant of the dimension of a length, which is called the "effective range" of the nuclear forces. The term of order  $k^4r_0^3$  is negligible at "classical"<sup>2</sup> neutron energies. Therefore, if  $\delta$  is obtained from experiment and  $k \cot \delta$  plotted against the neutron energy (i.e.,  $k^2$ ), a straight line will result. The slope of this line determines the effective range  $r_0$ ; the intercept at  $k=0$  gives the scattering length<sup>3</sup> at zero energy,  $a$ , by means of the relation

$$1/a \equiv \alpha = \gamma(1 - \frac{1}{2}\gamma r_0). \quad (3)$$

The singlet scattering can be treated in an analogous way.

It has long been suspected that "classical" nuclear scattering experiments can only determine two parameters in the nuclear potential, let us say an effective range and an effective depth. This was demonstrated with the greatest thoroughness by Breit and his collaborators<sup>4</sup> for proton-proton

scattering. For any reasonable shape of the nuclear potential, they could choose two parameters (depth and range) in such a way as to fit the observed scattering essentially within experimental error. This showed that practically no information could be obtained, from classical scattering experiments, on the shape of the potential. Subsequently, Landau and Smorodinsky<sup>5</sup> surmised the relations (12) and (51) which are similar to (1). However, Schwinger was the first to give a general proof of these relations.

Schwinger's proof is based on a variational principle and is quite complicated. It is the main purpose of this paper to give a greatly simplified derivation. Because of the simplicity, it is then easy to calculate higher terms in Eq. (1), and in particular to show generally that the neglected term is not only of order  $k^4$  but in addition has a very small coefficient. For the proton-proton scattering, a similar equation (Eq. (51)) can be derived with very little trouble; moreover, the relation between proton-proton and proton-neutron force can be established without explicit calculation of the nuclear potential. In a subsequent paper, it will be shown that the photoelectric and the photomagnetic effects of the deuteron can be calculated in terms of the effective ranges, and that the theory can be generalized to the case of tensor forces.

Blatt<sup>1</sup> has applied Schwinger's theory to an evaluation of the experiments on neutron-proton scattering. Blatt and Jackson<sup>6</sup> have analyzed all the implications of the theory and have, in addition, given very useful curves and formulas showing the relation between the parameters of potentials of

\* This work was done while the author was a Visiting Professor at Columbia University, New York, New York.

<sup>1</sup> J. Schwinger, Harvard lecture notes (photographed only). Quoted by J. Blatt, Phys. Rev. 74, 92 (1948). See reference 6, Sections 2 and 3.

<sup>2</sup> The expression "classical nuclear physics" was introduced by S. Allison to describe the energy region up to, say, 10 or 20 Mev.

<sup>3</sup> E. Fermi and L. Marshall, Phys. Rev. 71, 666 (1947).

<sup>4</sup> Breit, Thaxton, and Eisenbud, Phys. Rev. 55, 1018 (1939); Hoisington, Share, and Breit, Phys. Rev. 56, 884 (1939).

<sup>5</sup> Landau and Smorodinsky, J. Phys. Acad. Sci. U.S.S.R. 8, 154 (1944); Smorodinsky, J. Phys. Acad. Sci. U.S.S.R. 8, 219 (1944); 11, 195 (1947).

<sup>6</sup> J. M. Blatt and J. D. Jackson, Phys. Rev. this issue. Referred to as BJ. As far as possible, the same notation is used here as in BJ.

various shapes, and the effective range and scattering length. They have also evaluated the coefficient of  $k^4 r_0^3$  in (1) for various potential shapes. We shall therefore refer to their paper with regard to quantitative numerical results obtainable with the present theory.

## II. NEUTRON-PROTON SCATTERING, EFFECTIVE RANGE

Consider a neutron of energy  $E_1$  and wave number  $k_1$ . If  $E_1$  is in the laboratory system,

$$E_1 = 2\hbar^2 k_1^2 / M. \quad (4)$$

Let  $u_1$  by the radial wave function multiplied by  $r$ , for an  $S$  state; then  $u_1$  satisfies the Schrödinger equation

$$d^2 u_1 / dr^2 + k_1^2 u_1 - V(r) u_1 = 0, \quad (5)$$

where  $V$  is the potential energy, multiplied by  $M/\hbar^2$ . For another energy, we have

$$d^2 u_2 / dr^2 + k_2^2 u_2 - V(r) u_2 = 0. \quad (5a)$$

Multiply (5) by  $u_2$  and (5a) by  $u_1$ , subtract and integrate; then we get

$$u_2 u_1' - u_1 u_2' \Big|_0^R = (k_2^2 - k_1^2) \int_0^R u_1 u_2 dr, \quad (6)$$

where the upper limit  $R$  is arbitrary.

If  $R$  is infinity, the orthogonality relation results. If  $R$  is chosen equal to the range of the nuclear forces, one obtains the relation of Bethe and Peierls<sup>7</sup> between scattering phase shift and  $k$ . We shall not use (6) directly, but first introduce a comparison function  $\psi$  which represents the asymptotic behavior of  $u$  for large distances, *viz.*

$$\psi_1 = A_1 \sin(k_1 r + \delta_1), \quad (7a)$$

where  $\delta_1$  is the phase shift<sup>8</sup> for energy  $E_1$ . It is most convenient to choose the normalizing factor  $A_1$  so as to make  $\psi = 1$  at the origin, thus:

$$\psi_1 = \sin(k_1 r + \delta_1) / \sin \delta_1. \quad (7)$$

This will at the same time determine the normalization of  $u$  since  $u$  is supposed to approach  $\psi$  asymptotically for large  $r$  including normalization.

For the  $\psi$ 's, a relation analogous to (6) will hold, *viz.*:

$$\psi_2 \psi_1' - \psi_1 \psi_2' \Big|_0^R = (k_2^2 - k_1^2) \int_0^R \psi_1 \psi_2 dr. \quad (8)$$

Now subtract (6) from (8). Then, if the upper limit  $R$  is chosen large compared with the range of the nuclear forces, each function  $u_i$  will be equal to

<sup>7</sup> H. A. Bethe and R. E. Peierls, Proc. Roy. Soc. A148, 146 (1935).

<sup>8</sup> All considerations refer to  $S$  waves; therefore we do not need to put the orbital momentum in evidence by writing  $\delta_l$ . The subscript in this paper will generally refer to the energy, not to  $l$ .

its asymptotic form  $\psi$ , and there will therefore be no contribution to the integrated term (left-hand side) from the upper limit  $R$ . For the same reason, the integral on the right-hand side can now be extended to infinity. At the lower limit,  $u_1 = u_2 = 0$  so that this term does not contribute. This leaves

$$(\psi_2 \psi_1' - \psi_1 \psi_2')_{r=0} = (k_2^2 - k_1^2) \int_0^\infty (\psi_1 \psi_2 - u_1 u_2) dr. \quad (9)$$

Now we have normalized  $\psi$  to unity at  $r=0$  (Eq. (7)), and the derivative of  $\psi$  can easily be obtained from (7) so that we find

$$k_2 \cot \delta_2 - k_1 \cot \delta_1 = (k_2^2 - k_1^2) \int_0^\infty (\psi_1 \psi_2 - u_1 u_2) dr. \quad (10)$$

This equation is exact and is the fundamental equation of our theory.

We can now apply (10) to the special case  $k_1 = 0$ . Then

$$k_1 \cot \delta_1 = -\alpha \equiv -1/a, \quad (11)$$

where  $a$  is the scattering length of Fermi and Marshall, for zero-energy neutrons, which can be determined with great accuracy. For the triplet state,  $a$  is positive, for the singlet state, negative. We shall use subscripts zero for the wave functions referring to zero energy, and we may drop the subscripts for state 2. Then (10) becomes

$$k \cot \delta = -\alpha + \frac{1}{2} k^2 \rho(0, E) \quad (12)$$

with

$$\frac{1}{2} \rho(0, E) = \int_0^\infty (\psi_0 \psi - u_0 u) dr. \quad (13)$$

Clearly,  $\rho$  has the dimension of a length. It can also be defined for two arbitrary energies,

$$\frac{1}{2} \rho(E_1, E_2) = \int_0^\infty (\psi_1 \psi_2 - u_1 u_2) dr. \quad (13a)$$

The important point is now that  $\psi$  and  $u$  differ only inside the range of the nuclear forces. Therefore the integrands in (13) and (13a) will be different from zero only inside the force-range. However, in this region the wave functions  $u$  and  $\psi$  depend only very slightly on energy, because  $kr$  is small and the potential energy is much larger than  $k^2$ . Therefore it will be a good approximation (indeed a very good one, as we shall show in the next section) to replace  $u$  by  $u_0$  and  $\psi$  by  $\psi_0$  and to write

$$\frac{1}{2} \rho(0, E) \approx \frac{1}{2} \rho(0, 0) = \frac{1}{2} r_0 = \int_0^\infty (\psi_0^2 - u_0^2) dr. \quad (14)$$

This quantity is now a constant, independent of energy, and we call it the *effective range*.<sup>9</sup> It is

<sup>9</sup> F. C. Barker and R. E. Peierls, Phys. Rev. 75, 312 (1949), have given a similar derivation for the effective range. Also similar are the calculations of G. F. Chew and M. L. Goldberger, Phys. Rev. 75, 1637 (1949).

identical with the effective range used and defined by Blatt and Jackson. (For the shape of the functions  $\psi_0$  and  $u_0$  see their Fig. 3.) Schwinger defined  $r_0$  by

$$\frac{1}{2}r_0 = \int_0^\infty (\psi_g^2 - u_g^2) dr, \quad (14a)$$

where  $u_g$  and  $\psi_g$  refer to the ground state of the deuteron, and in particular  $\psi_g$  is the asymptotic solution

$$\psi_g = e^{-\gamma r} \quad (15)$$

with  $\gamma$  defined in (2). Since  $\rho(E_1, E_2)$  is insensitive to the energies  $E_1$  and  $E_2$ , it makes little difference if both of them are replaced by  $-\epsilon$  where  $\epsilon$  is the binding energy of the deuteron; so Schwinger's effective range is very close to ours. Blatt and Jackson have shown that (14) will give a somewhat closer approximation to the scattering than (14a).

Using (14), then, the fundamental relation (12) reduces to

$$k \cot \delta = -\alpha + \frac{1}{2}k^2 r_0. \quad (16)$$

Schwinger's relation (1) is obtained from (10) if the comparison state is taken to be the ground state. As pointed out by Blatt, and mentioned in the Introduction, these relations are both very convenient for the analysis of neutron-proton scattering data, although some complication is caused by the mixture of triplet and singlet scattering. If these two parts can be separated and  $\delta$  determined for triplet and singlet separately, a straight line is obtained when the empirically determined quantity  $k \cot \delta$  is plotted against the "energy"  $k^2$ .

Equation (16) may be inserted in the formula for the cross section,

$$\frac{\sigma}{4\pi} = \frac{\sin^2 \delta}{k^2} = \frac{1}{k^2 + k^2 \cot^2 \delta} = [k^2 + \alpha^2 - k^2 \alpha r_0 + \frac{1}{4}k^2 r_0^2 + O(k^2 \alpha r_0^2)]^{-1}. \quad (17)$$

Actually, the more complicated Schwinger expression (1) gives a simpler result because several terms combine, *viz.*

$$\sigma = \frac{4\pi}{(k^2 + \gamma^2)} [1 - \gamma r_0 + \frac{1}{4}(k^2 + \gamma^2)r_0^2 + O(k^2 \gamma r_0^2)]^{-1}. \quad (18a)$$

Thus, in first approximation, the cross section is multiplied by the constant factor  $1/(1 - \gamma r_0)$  as already pointed out by Bethe and Peierls. But the following correction term,  $\frac{1}{4}(k^2 + \gamma^2)r_0^2$ , while in general much smaller than the first, still is unaffected by the omission of higher order corrections in (16) or (1): these neglected terms will only give contributions of relative order  $(kr_0)^2$ . Schwinger has pointed out that the term in  $(kr_0)^2$  is required

in order to keep the cross section everywhere below the permitted maximum,  $4\pi/k^2$ . This maximum is reached when  $\cot \delta = 0$ , i.e.,  $k^2 = 2\alpha/r_0$ . For triplet scattering, with the numerical values given in the next section, this corresponds to 20 Mev neutron energy (laboratory system).

### III. DETERMINATION OF RANGE FROM PARA-HYDROGEN SCATTERING

If the state 2 in (10) is taken to be the ground state, then from (15) we have  $\psi_2'(0) = -\gamma$ , and we find

$$\alpha = \gamma - \frac{1}{2}\gamma^2 \rho(0, -\epsilon) \approx \gamma(1 - \frac{1}{2}\gamma r_0), \quad (19)$$

which is also contained in the Schwinger relation (1). This provides the most accurate way to determine  $r_0$  for the triplet state<sup>1,6</sup> because  $\gamma$  is known from the binding energy of the deuteron and  $\alpha$  from the parahydrogen scattering.

Since all the relevant experimental data are still subject to correction, it is desirable to indicate the change of the result which would be caused by a given change of the experimental numbers. We put: Binding energy of deuteron

$$\epsilon = 2.21(1 + \epsilon_1) \text{ Mev.} \quad (20a)$$

Scattering cross section of slow neutrons by free protons  $\sigma_f = 20.36(1 + \epsilon_2) \text{ barns.}$  (20b)

Scattering of parahydrogen

$$(3a_t + a_s)^2 = 0.624(1 + \epsilon_3) \text{ barns,} \quad (20c)$$

where  $a_t$  and  $a_s$  are the scattering lengths for triplet and singlet, respectively, so that

$$\sigma_f = \pi(3a_t^2 + a_s^2). \quad (21)$$

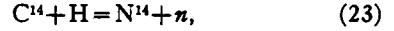
The corrections  $\epsilon_1$ ,  $\epsilon_2$ ,  $\epsilon_3$  may be just as easily positive as negative; the present indicated probable errors are about

$$\epsilon_1 = \pm 0.009 \quad (\pm 20 \text{ kev}), \quad (22a)$$

$$\epsilon_2 = \pm 0.005 \quad (\pm 0.10 \text{ barn}), \quad (22b)$$

$$\epsilon_3 = \pm 0.08 \quad (\pm 0.050 \text{ barn}). \quad (22c)$$

The value for the binding energy of the deuteron is taken<sup>10</sup> mainly from the reaction



whose threshold has been accurately determined by Shoupp and Jennings<sup>11</sup> giving  $Q = -620 \pm 9$  kev. The energy of the  $\beta$ -rays from  $C^{14}$  is extremely well known, e.g., from the measurement of Langer,

<sup>10</sup> I am indebted to Dr. K. Bainbridge for a discussion of the experimental information on the deuteron binding energy at the Conference on Classical Nuclear Physics at Chicago, December 1948. Dr. Bainbridge will publish a more detailed discussion in the near future.

<sup>11</sup> Shoupp, Jennings, and Sun, Phys. Rev. 75, 1 (1949).

Cook, and Price,<sup>12</sup> and is  $156.3 \pm 1.0$  kev. This gives for the difference†

$$n - H = 776 \pm 9 \text{ kev.} \quad (23a)$$

Combining this with the mass spectrograph doublet

$$H_2 - D = 1432 \pm 2 \text{ kev,} \quad (23b)$$

we get for the binding energy of the deuteron

$$n + H - D = \epsilon = 2208 \pm 7 \text{ kev.} \quad (23c)$$

Probably the best *direct* measurement of the binding energy is the recent one by Bell and Elliot<sup>13</sup> at Chalk River who measured the energy of the  $\gamma$ -rays from the capture reaction and found

$$\epsilon = 2237 \pm 5 \text{ kev} \quad (24)$$

referred to the ThC''  $\gamma$ -ray which was taken as 2620 kev. Since this involves an absolute calibration of  $\gamma$ -ray energies<sup>14</sup> and since (23a) involves only the measurement of small energies, we shall provisionally adopt (23c) until the small discrepancy between it and (24) is resolved. In any case, the lower values (2185 kev) found earlier<sup>15</sup> seem to be discredited.

For the free proton cross section, we take the very accurate value obtained by Melkonian, Rainwater and Havens<sup>16</sup> with the Columbia velocity selector. For the parahydrogen scattering, the value of Sutton *et al.*<sup>17</sup> obtained at Los Alamos was taken; a relatively generous probable error seemed indicated (see the discussion in BJ, Section VI).

The values chosen in (20) give for the "radius of the deuteron"

$$1/\gamma = 4.332(1 + \frac{1}{2}\epsilon_1) \times 10^{-13} \text{ cm} \quad (25)$$

for the two scattering lengths

$$-a_s = (2.375 + 1.11\epsilon_2 + 0.072\epsilon_3) \times 10^{-12} \text{ cm,} \quad (26a)$$

$$a_t = (0.528 + 0.37\epsilon_2 - 0.108\epsilon_3) \times 10^{-12} \text{ cm,} \quad (26b)$$

and, using (19), for the effective range

$$r_0 = (1.56 + 2.7\epsilon_1 + 5.0\epsilon_2 - 1.5\epsilon_3) \times 10^{-13} \text{ cm.} \quad (27)$$

<sup>12</sup> Cook, Langer, and Price, Phys. Rev. 74, 548 (1948).

† Note added in proof.—Recent measurements by Taschek, Jarvis, Argo, and Hemmendinger (Phys. Rev. 75, 1268 (1949)) and by Tollestrup, Jenkins, Fowler, and Lauritsen (Phys. Rev. 75, 1947 (1949) and private communication) on the difference  $He^3 + n - H^2 - H$  give values for  $n - H$  of  $782 \pm 2$  kev and  $789 \pm 6$  kev, respectively, which would slightly raise  $\epsilon$  if (23b) is correct. However, this does not resolve the discrepancy pointed out in footnote 14.

<sup>13</sup> R. E. Bell and L. G. Elliot, Phys. Rev. 48, 1552 (1948).

<sup>14</sup> T. Lauritsen has informed the author that he has re-determined the energy of the ThC''  $\gamma$ -ray by direct comparison with annihilation radiation, and found  $2618 \pm 5$  kev. This would indicate a definite discrepancy between (23c) and (24).

<sup>15</sup> See the review by W. E. Stephens, Rev. Mod. Phys. 19, 19 (1947).

<sup>16</sup> Melkonian, Rainwater, and Havens, Phys. Rev. 75, 1295 (1949).

<sup>17</sup> Sutton, Hall, Anderson, Bridge, DeWire, Lavatelli, Long, Snyder, and Williams, Phys. Rev. 72, 1147 (1947).

Inserting (22), we find for the contributions to the uncertainty of the effective range:

from the deuteron binding energy  $0.024 \times 10^{-13}$ , (27a)

from the free-proton scattering  $0.025 \times 10^{-13}$ , (27b)

from the parascattering  $0.12 \times 10^{-13}$ . (27c)

As is to be expected, the parascattering gives the greatest uncertainty and more precise experiments are very desirable. An additional uncertainty arises from the slight difference between  $\rho(0, -\epsilon)$  and  $\rho(0, 0)$  which depends on the shape of the potential; from Fig. 14 of BJ this effect may be estimated to be an increase of  $r_0$  by about 0.01 for the square well, and a decrease of about 0.04 for the Yukawa potential, as compared with the value given in (27).

The singlet scattering range cannot be deduced with any certainty from existing neutron-proton experiments (BJ Fig. 8). The best procedure still seems to be to assume approximate equality of force in the singlet state for proton-proton and neutron-proton. The proton-proton data (Section 6) give  $r_0 = 2.7 \times 10^{-13}$  which we shall assume to be true also for neutron-proton singlet scattering. This means a large difference between the effective ranges for triplet and singlet states. Now for square wells the effective range is nearly equal to the actual width (intrinsic range) of the square well and therefore the intrinsic ranges come out very differently for triplet and singlet (1.85 and  $2.55 \times 10^{-13}$ , respectively). But for long-tailed potentials, there is a large difference between intrinsic and effective range, especially for the triplet state which is relatively strongly bound. For such potentials, then, the same intrinsic range may easily be compatible with the observed large difference in effective ranges in singlet and triplet states. This is true, in particular, for a Yukawa potential if the intrinsic range is chosen to be

$$b_s = b_t = 2.5 \times 10^{-13} \text{ cm.} \quad (28)$$

That it is possible to use the same intrinsic potential for triplet and singlet, is due to the fact that the "Yukawa" curve for  $b/r_0$  vs.  $a\tau_0$ , Fig. 6 of BJ, is very steep when  $a\tau_0$  is large which it is for the triplet state, *viz.* about 0.3 from Eq. (26b) and (27). Therefore almost any value of  $b_s$  is compatible with a given  $r_0$ , and among them also  $b_t$ . It is therefore better to turn the argument around and assume  $b_s = b_t$  to be given by (28), and  $r_t$  by (27), then we get  $b_t/r_t = 1.6$ ; and from BJ Fig. 6 we find  $a\tau_t = r_t/a_s = 0.28$  in good agreement with (26b), (27). Thus, if we knew (a) that the potential had a Yukawa shape and (b) that  $ab$  is rather large, we could predict the effective triplet range quite accurately from the scattering length  $a_s$  alone,

without knowing the binding energy of the ground state; or we might even predict  $r_t$  and  $a_t$  (and thus the parahydrogen scattering) directly from the binding energy of the deuteron, using  $\alpha r_0 \approx 0.3$  and Eq. (19).

The fact that the small effective triplet range is compatible with a large singlet range for a long-tailed potential, is the reason why Bohm and Richman<sup>18</sup> found it possible to explain the observed neutron-proton scattering up to 6 Mev with the same well for singlet and triplet *provided* they took a long-tailed well.

#### IV. ENERGY DEPENDENCE OF EFFECTIVE RANGE

We shall now study the dependence on energy of  $\rho(0, E)$ , as defined by Eq. (13). For this purpose we expand the comparison function  $\psi$  up to second order in  $k$ ; we get from (7)

$$\begin{aligned}\psi &= \cos kr + \cot \delta \sin k \\ &= 1 - \frac{1}{2}k^2r^2 + k \cot \delta r - \frac{1}{6}k^3 \cot \delta r^3 + O(k^4r^4).\end{aligned}\quad (29)$$

Now we insert for  $k \cot \delta$  the first approximation (16) which is also accurate including terms of order  $k^2$ ; then

$$\psi = 1 - \alpha r + \frac{1}{2}k^2r(r_0 - r) - \frac{1}{6}k^2\alpha r^3. \quad (29a)$$

The first two terms are independent of energy, the other two are proportional to the energy. It is often convenient to write  $\psi$  in the form

$$\psi = \psi_0 + k^2\chi_1 + k^4\chi_2 + \dots \quad (30)$$

Then, according to (29a),

$$\chi_1 = \frac{1}{2}r(r_0 - r) - \frac{1}{6}\alpha r^3. \quad (30a)$$

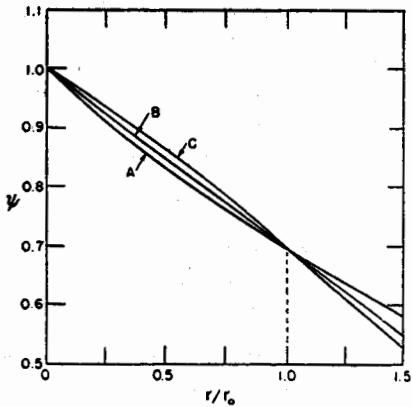


FIG. 1. The comparison functions  $\psi$  vs. radius for (A) the ground state of the deuteron, (B) the triplet state of energy zero, and (C) a neutron whose kinetic energy in the laboratory system is twice the binding energy. All curves intersect at the effective range  $r_0$ .

<sup>18</sup> D. Bohm and C. Richman, Phys. Rev. 71, 567 (1947). This fact was pointed out to the author by Dr. Blatt.

This function is zero at  $r=0$  because all  $\psi$ 's are normalized to unity at this point; then it becomes positive because  $k \cot \delta$  (the slope of  $\psi$ ) increases with energy;  $\chi_1$  has a negative curvature which arises from the term  $\cos kr$  in (29); therefore it becomes zero again, at

$$r \equiv r_1 \approx r_0(1 - \frac{1}{3}\alpha r_0) \quad (31)$$

which is rather close to  $r_0$ , and is negative thereafter. In this approximation, then, the functions  $\psi$  for all energies will intersect near the effective range. (See Fig. 1.)

The energy dependent term  $\chi_1$  is obviously small for any value of  $r$  comparable with  $r_0$ , i.e., anywhere within the range of the nuclear forces, whatever their shape. This is because  $\chi_1$  has two zeros, one at 0 and one at  $r_1$  and is therefore a small fraction of  $r_0^2$  in the interesting range. Therefore  $\psi - \psi_0$  will be a small numerical coefficient multiplied by  $(kr_0)^2$  which itself is small for energies up to 10 Mev or so. We shall see that this makes the simple theory of Section II such a good approximation.

The correction to the simple theory is given by

$$\begin{aligned}\frac{1}{2}\rho(E, 0) - \frac{1}{2}\rho(0, 0) &= \int [\psi_0(\psi - \psi_0) - u_0(u - u_0)] dr \\ &= k^2 \int_0^\infty (\psi_0 \chi_1 - u_0 v_1) dr,\end{aligned}\quad (32)$$

if we set, in analogy to (30),

$$u = u_0 + k^2 v_1 + k^4 v_2 + \dots \quad (32a)$$

The first part of (32), the integral of  $\psi_0 \chi_1$ , is small because  $\chi_1$  has been shown to be small (compared with  $r_0^2$ ) inside the range of the nuclear forces. The function  $v_1$  must also be small in this region because it must approach  $\chi_1$  as soon as the nuclear forces become negligible, and must be zero for  $r=0$ . Therefore the factor of  $k^2$  in (32) must be small compared with  $r_0^3$ .

BJ have written the phase shift formula in the form

$$k \cot \delta = -\alpha + \frac{1}{2}k^2 r_0 - P k^4 r_0^3 + \dots \quad (33)$$

Our argument then shows that  $P$  must be a small numerical coefficient. This is indeed what BJ find by explicit calculation. According to their Fig. 10,  $P$  is in most cases less than 0.05 and never exceeds 0.14. It depends, of course, on the shape of the potential and on the quantity  $\alpha r_0$ ; see Eq. (11).

It is very easy to calculate  $P$  for a square well, especially if we assume the resonance level to lie exactly at zero energy, i.e., if  $\alpha=0$ . Then  $\psi_0$  is equal to unity,  $\alpha$  is zero,  $r_0$  is equal to the actual width  $b$  of the well, and  $\chi_1$  is positive throughout the region contributing to the integral in (32). The first term

in this integral then gives

$$\int_0^{r_0} \psi_0 \chi_1 dr = \frac{1}{2} \int_0^{r_0} r(r_0 - r) dr = \frac{1}{12} r_0^3. \quad (34)$$

The factor here is indeed small. Moreover, the second term in the integral (32) has always the opposite sign and is in general smaller than the first (since  $u_0 \leq \psi_0$  everywhere); so the actual result of (32) will be even smaller than that obtained from the first term alone. Explicitly, we have for the square well

$$u_0 = \sin Kr, \quad K = \pi/2b, \quad (35a)$$

$$u = \sin[(K^2 + k^2)^{1/2}r], \quad (35b)$$

$$v_1 = (u - u_0)/k^2 = (r/2K) \cos Kr, \quad (35c)$$

$$\int_0^{r_0} u_0 v_1 dr = r_0^3/2\pi^2. \quad (35)$$

This is indeed of the same sign, and smaller than, Eq. (34). Combining them we get

$$\rho(0, k^2) = r_0 + 0.0654k^2r_0^3 \quad (36)$$

$$P = -0.0327. \quad (36a)$$

The correction to the effective range is very small. For 10 Mev and the observed value of  $r_0$ , Eq. (27), we have  $kr_0 = 0.54$  and the second term of (36) is 2 percent of the first. The effect on the phase shift is about  $0.3^\circ$ . This shows the excellence of the simple (Schwinger) approximation given by Eq. (16).

We have seen that the correction function  $\chi_1$  is positive for  $r < r_1 \approx r_0$ , negative for  $r > r_1$ . Therefore the correction term (32) is positive for the square well where the entire contribution comes from  $r < r_1$ . On the other hand, for a long-tailed potential such as that of Yukawa, most of the contribution to (32) is likely to come from  $r > r_1$ , where  $\chi_1$  is negative, especially because  $|\chi_1|$  is on the whole greater for  $r > r_1$ . Therefore we should expect that the correction term (32) is negative ( $P$  positive) for long-tailed potentials. BJ have shown that this is indeed the case for the Yukawa and the exponential potential.

Another factor which tends to make (32) negative is that in this case  $v_1$  is algebraically larger than  $\chi_1$  so that the second term in (32) gives an additional negative contribution. (For the square well,  $v_1$  is algebraically smaller than  $\chi_1$ .) This is illustrated in Fig. 2. This argument, as well as the calculations for Fig. 2, are due to Dr. C. Longmire.

The coefficient  $P$  is the first parameter in the expansion (33) of  $k \cot \delta$  which depends on the shape of the potential. If the scattering experiments could be made accurate enough to deduce  $P$ ,

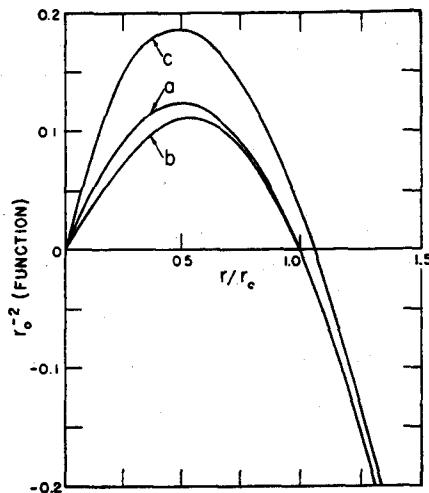


FIG. 2. The energy-dependent corrections to the wave function vs. radius (a) the correction  $\chi_1 = d\psi/dk^2$  to the comparison function, (b) the correction  $v_1 = du/dk^2$  to the actual wave function for a square well, (c)  $v_1$  for a Yukawa potential. In b and c, the energy of the resonance level was assumed to be zero.

information on the shape would be obtained. If the plot of  $k \cot \delta$  vs.  $k^2$  deviates from a straight line upwards we have a concentrated potential (square well or Gaussian); if the deviation is downwards the potential has a long tail (exponential or Yukawa potential). For the present, the experimental accuracy is not sufficient to make any deviations from the straight line significant. The only arguments for the shape of the potential are then of the type presented in the last section, *viz.* that the Yukawa potential permits the intrinsic range to be the same for triplet and singlet, while the square well would require very different intrinsic ranges in the two cases. From the triplet or the singlet scattering separately, each as a function of energy, nothing could be said about the shape. Moreover, to predict the scattering at an energy where it has not been measured, the straight line relation (16) appears to be the simplest as well as a very accurate method.

#### V. PROTON-PROTON SCATTERING: THEORY

In the case of proton-proton scattering, the Coulomb potential is added to the nuclear interaction. If  $w_1$  is the radial wave function multiplied by  $r$ , for wave number  $k_1$ , then

$$w_1'' + k_1^2 w_1 = V w_1 + 2w_1/Dr. \quad (37)$$

The last term represents the Coulomb potential, and  $D$  is the Bohr radius for two protons,

$$D = 2\hbar^2/Mc^2 = 5.76 \times 10^{-12} \text{ cm} \quad (38)$$

(factor 2 because of reduced mass). Because of the relative smallness of the Coulomb potential, the

Bohr radius  $D$  is very large compared with nuclear dimensions. This will be useful in the analysis.

We use again a comparison function,  $\varphi$ , which is the solution in the Coulomb field alone, *viz.*

$$\varphi_1'' + k_1^2 \varphi_1 = 2\varphi_1/D. \quad (39)$$

It is so chosen that  $w$  becomes equal to  $\varphi$  asymptotically, i.e., outside the range of the nuclear forces. The function  $\varphi$  itself is quite complicated but most of its relevant properties, as well as tables, have been given by Yost, Wheeler, and Breit.<sup>20</sup> For  $kr \gg 1$ ,  $\varphi$  has the asymptotic form

$$\varphi = C \sin(kr - \eta \log 2kr + 2 \arg \Gamma(1+i\eta) + \delta_1), \quad (40)$$

where  $C$  is a normalizing constant,

$$\eta = e^2/\hbar v = 1/kD = (25.0 \text{ kev}/E)^{\frac{1}{2}} \quad (41)$$

is a very useful parameter, and  $\arg \Gamma$  is the complex phase of the  $\Gamma$ -function,

$$\Gamma(x) = |\Gamma(x)| \exp[i \arg \Gamma(x)]. \quad (41a)$$

The phase shift relative to the regular Coulomb function is denoted by  $\delta$  (Breit's  $K_0$ ). The function  $\varphi$ , like its counterpart  $\psi$  in Section II, shall be normalized to unity at  $r=0$ . It can then be expressed, at any value of  $r$ , by a combination of regular and irregular solutions in the Coulomb potential which are denoted by  $F$  and  $G$ , respectively, by YWB, thus:

$$\varphi = C_0(G + F \cot \delta), \quad (42)$$

where  $C_0$  is the well-known normalizing constant for Coulomb wave functions,

$$C_0 = \left( \frac{2\pi\eta}{e^{2\pi\eta} - 1} \right)^{\frac{1}{2}}. \quad (43)$$

As before, the normalization of  $\varphi$  determines that of  $w$ .

Then, using a proof entirely analogous to Section II, we get

$$\begin{aligned} & \varphi_1 \varphi_1' - \varphi_1 \varphi_2' - w_1 w_1' + w_1 w_2' \Big|_r^R \\ &= (k_2^2 - k_1^2) \int_r^R (\varphi_1 \varphi_2 - w_1 w_2) dr. \quad (44) \end{aligned}$$

The only difference as compared with Section II is that we now take a *finite* lower limit  $r$ , which, however, we assume to be very small compared with  $r_0$ . The integrated term in (44) is again zero at the upper limit; at the lower limit, the functions  $w$  are zero and the  $\varphi$ 's are 1 (within corrections of order

<sup>20</sup> Yost, Wheeler, and Breit, Phys. Rev. 49, 174 (1937). Quoted as YWB.

$r$ ). Then we get

$$\begin{aligned} \varphi_2'(r) - \varphi_1'(r) &= (k_2^2 - k_1^2) \int_r^\infty (\varphi_1 \varphi_2 - w_1 w_2) dr \\ &= \frac{1}{2}(k_2^2 - k_1^2)\rho(E_1, E_2) \quad (45) \end{aligned}$$

in complete analogy with (10), (13a). Equation (45) defines the "effective range"  $\rho$ .

We must now investigate the derivative  $\varphi'(r)$ . For small but finite  $r$ , YWB give for the irregular function

$$\begin{aligned} C_0 G &= 1 + \frac{2r}{D} \left( \ln \frac{2r}{D} - \ln \eta \right. \\ &\quad \left. + R.P. \Psi(i\eta) + 2C - 1 \right) + O(r^2), \quad (46) \end{aligned}$$

where  $C$  is Euler's constant,  $0.577\dots$  and  $\Psi$  the logarithmic derivative of the  $\Gamma$ -function.

$$\Psi(z) = \frac{\Gamma'(z+1)}{\Gamma(z+1)} = \sum_{n=1}^{\infty} \left( \frac{1}{n} - \frac{1}{z+n} \right) - C \quad (46a)$$

so that

$$R.P. \Psi(i\eta) + C = \eta^2 \sum_{n=1}^{\infty} \frac{1}{n(n^2 + \eta^2)}. \quad (46b)$$

Further evaluations are given by YWB. For reasonably high energy ( $> 0.5$  Mev) it is sufficient to set

$$R.P. \Psi(i\eta) + C = \eta^2 s_3, \quad s_3 = \sum_{n=1}^{\infty} n^{-3} = 1.202. \quad (46c)$$

We abbreviate

$$C_0 G = 1 + (2r/D)[\ln(2r/D) + \frac{1}{2}g(\eta) + C - 1], \quad (47)$$

where  $g$  is a known function of  $\eta$ , *viz.*

$$g = -2 \ln \eta + 2\eta^2 \sum_{n=1}^{\infty} n^{-1} (n^2 + \eta^2)^{-1}. \quad (47a)$$

The regular function is, up to order  $r$ , simply

$$F = C_0 kr \quad (48)$$

and therefore

$$\begin{aligned} \varphi &= C_0(G + F \cot \delta) \\ &= 1 + (2r/D)[\ln(2r/D) + \frac{1}{2}g(\eta) + C - 1 \\ &\quad + \frac{1}{2}C_0^2 k D \cot \delta] \\ &= 1 + \frac{2r}{D} \left[ \ln \frac{2r}{D} + \frac{1}{2}g(\eta) + C - 1 + \frac{\pi \cot \delta}{e^{2\pi\eta} - 1} \right]. \quad (49) \end{aligned}$$

where the values of  $C_0$ , (42), and of  $\eta$ , (41), have been inserted.

It is seen that  $\varphi'$  is logarithmically infinite for  $r=0$ . Therefore the direct use of  $\varphi'(0)$  is impossible,

and it is for this reason that we had to use a finite lower limit  $r$  in (45). But if we take the difference of the values of  $\varphi'$  for two different energies,  $E_2$  and  $E_1$ , and at the same  $r$ , the troublesome term  $\log r$  cancels out since it is energy-independent. We get then from (45), (49) :

$$\begin{aligned}\varphi_2' - \varphi_1' &= \frac{1}{D} \left[ g(\eta_2) - g(\eta_1) + \frac{2\pi \cot \delta_2}{e^{2\pi\eta_2} - 1} - \frac{2\pi \cot \delta_1}{e^{2\pi\eta_1} - 1} \right], \\ &= \frac{1}{2}(k_2^2 - k_1^2)\rho(E_1, E_2),\end{aligned}\quad (50)$$

or, putting  $k_1 = 0$ :

$$f \equiv g(\eta) + \frac{2\pi \cot \delta}{e^{2\pi\eta} - 1} = D[-\alpha' + \frac{1}{2}k^2\rho(0, E)], \quad (51)$$

where  $\alpha'$  is a constant, independent of energy, and analogous to the reciprocal scattering length  $\alpha$  in (16).

Equation (51) is quite similar to (16). It also was obtained by Schwinger<sup>1</sup> from a variational principle. Previously, the relation had been stated but not proved by Landau and Smorodinsky. The quantity  $f$  itself was already defined and found useful by Breit, Condon, and Present<sup>2</sup> in their first theory of the proton-proton scattering. These authors pointed out that  $f$  should be independent of energy if the range of the nuclear forces were zero, and derived the consequences of such an assumption for the behavior of  $\delta$  as a function of energy.

The left-hand sides of (51) and (50) differ from (16) in two respects: first, the factor of  $\cot \delta$  is not

simply  $k$  but (in (50))

$$\frac{2\pi}{D(e^{2\pi\eta} - 1)} = k \frac{2\pi\eta}{e^{2\pi\eta} - 1}. \quad (51a)$$

For large energies,  $\eta$  becomes small and this expression goes over into  $k$ , as it should. For small energies (large  $\eta$ ), however, the denominator becomes very large and consequently  $\cot \delta$  approaches infinity ( $\delta \rightarrow 0$ ) much more rapidly than for neutron-proton scattering. Physically this means the elimination of nuclear scattering by the Coulomb potential barrier.

The second difference is the appearance of the given function  $g(\eta)$  on the left side of (50) and (51).

On the right-hand side, the definition of  $\rho$  is the same as for neutron-proton scattering. Therefore the same arguments hold as there:  $\rho$  is very nearly independent of the energy, and may therefore be replaced by  $\rho(0, 0)$  which may again be called the effective range. Moreover, the Coulomb potential also has very little influence on the wave functions inside the range of the nuclear forces; therefore we may in good approximation replace  $\varphi, w$  by the functions  $\psi, u$  obtained in the same nuclear potential without Coulomb potential (see also Section VII). Then the effective range is defined by

$$\frac{1}{2}r_0 = \int_0^\infty (\varphi_0^2 - w_0^2)dr \approx \int_0^\infty (\psi_0^2 - u_0^2)dr, \quad (52)$$

where the subscript 0 again refers to zero energy, just as for neutron-proton scattering.

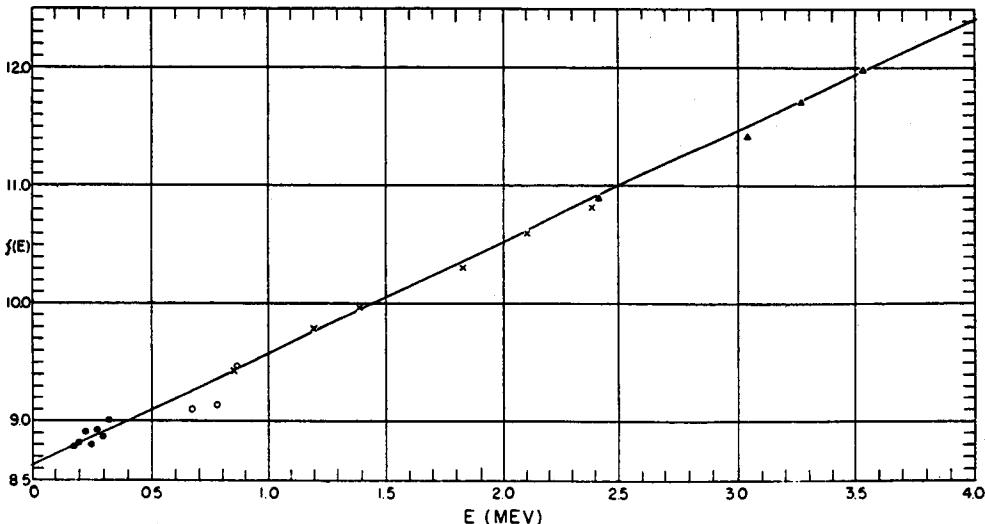


FIG. 3. Experiments on proton-proton scattering up to 4 Mev. The function  $f$ , Eq. (51), is plotted vs. energy. The experimental points fall very accurately on a straight line, as the theory predicts.

● Ragan, Kanne, and Taschek; ○ Heydenburg, Hafstad, and Tuve; × Herb, Kerst, Parkinson, and Plain;

△ Blair, Freier, Lampi, Sleator, and Williams.

<sup>1</sup> Breit, Condon, and Present, Phys. Rev. 50, 825 (1936).

TABLE I. Proton-proton phase shifts.

Energy (kev)	176.5	200.2	225.9	249.5	275.3	298.3	321.4
Reference							
$R^*$	0.544	0.448	0.353	0.256	0.177	0.118	0.070
$\delta$ (degrees)	5.77	6.78	7.85	9.03	10.05	10.97	11.83
Energy (Mev)	2.42	3.04	3.27	3.53			
Reference							
$R$	44.1	63.0	69.0	77.5			
$\delta$	48.17	51.17	51.50	52.08			
Energy		8.0		14.5			
Reference							
$\sigma_{e.m.}(90^\circ)^{**}$		6.0 ± 0.35		3.34 ± 0.2			
		52.6		52.0			

\*  $R$  is the ratio of observed scattering at  $45^\circ$  to Mott scattering.

\*\* Differential cross section in center of mass system.

## VI. ANALYSIS OF PROTON-PROTON SCATTERING EXPERIMENTS

To analyze the many accurate experiments on proton-proton scattering, we merely need to take the phase shifts of the  $s$ -wave from experiment, calculate the left-hand side of Eq. (51), and plot it against the energy. This has been done in Fig. 3.

It is seen that the experimental points fall very accurately on a straight line, as (51) demands. The line was actually drawn through the lowest energy points of Ragan, Kanne, and Taschek<sup>22</sup> (at 176 and 200 kev) and through the highest energy points of Blair, Freier, Lampi, Sleator, and Williams<sup>23</sup> (3.27 and 3.53 Mev). Then the points of Herb, Kerst, Parkinson, and Plain<sup>24</sup> fall very beautifully on the straight line. Only those of Hafstad, Heydenburg, and Tuve<sup>25</sup> are off the line, as was noticed before by Breit *et al.* and as is explainable from the early date at which this work was done, and from the fact that the electrostatic generator was pushed to the limit in energy.

For the two latter sets of experiments, I took the phase shifts from the work of Breit, Thaxton, and Eisenbud.<sup>4</sup> For the former two, they were evaluated by Longmire, using only the absolute scattering cross section at  $45^\circ$ . We realize that this is not the most accurate method of evaluation but it is simple and quick. The phase shifts obtained by Longmire, and used in constructing Fig. 3, are given in Table I.

The slope of the line in Fig. 3 is

$$0.942 \text{ per Mev} \quad (53a)$$

with an accuracy of 5 percent or better. Using  $D$  from (38), and (see (4))

$$E(\text{Mev}) = 0.830k^2(\text{barn}^{-1}), \quad (53b)$$

<sup>22</sup> Ragan, Kanne, and Taschek, Phys. Rev. 60, 628 (1941).

<sup>23</sup> Blair, Freier, Lampi, Sleator, and Williams, Phys. Rev. 74, 553 (1948).

<sup>24</sup> Herb, Kerst, Parkinson, and Plain, Phys. Rev. 55, 998 (1939).

<sup>25</sup> Heydenburg, Hafstad, and Tuve, Phys. Rev. 56, 1018 (1939).

we get the effective range

$$(2.71 \pm 0.13) \times 10^{-13} \text{ cm.} \quad (53)$$

This is in complete agreement with the analysis by Breit and collaborators. The limits on  $r_0$  can now be set considerably closer than by Breit, Thaxton, and Eisenbud, primarily because of the extension of the experiments to lower and higher energies, and to some extent because the very simple linear relation used here permits a very easy estimate of error by inspection.

The intrinsic range is slightly smaller than the effective range since the "level" of the proton-proton system is virtual. Using the scattering lengths given in Section VII, Eqs. (65) and (70), together with Fig. 6 of BJ, one obtains

$$b = 2.55 \times 10^{-13} \text{ for square well} \quad (54a)$$

$$b = 2.45 \times 10^{-13} \text{ for Yukawa potential.} \quad (54b)$$

Experiments on proton-proton scattering have also been done at higher energy, by Dearnley, Oxley, and Perry<sup>26</sup> and by R. R. Wilson and collaborators.<sup>27</sup> These are not as accurate as those at lower energy. However, we have plotted them in Fig. 4, together with the continuation of the straight line of Fig. 3. The agreement is not very good. In the case of the experiments of Wilson *et al.* the deviation is easily within the given experimental error. However, the point of Dearnley *et al.* is definitely off the straight line. The deviation is in the direction expected for a square well, while all other arguments favor something similar to a Yukawa potential. Moreover, the deviation is 4 times as great as expected for a square well. In fact, it was already noticed by Dearnley *et al.* that their cross section was lower (therefore  $k \cot \delta$  larger) than would be expected from the square well used by Breit *et al.* to fit the

<sup>26</sup> Dearnley, Oxley, and Perry, Phys. Rev. 73, 1290 (1948); (7 Mev).

<sup>27</sup> R. R. Wilson and E. Creutz, Phys. Rev. 71, 339 (1947); (8 Mev). Robert R. Wilson, Phys. Rev. 71, 384 (1947); (10 Mev). Wilson, Lofgren, Richardson, Wright, and Shankland, Phys. Rev. 72, 1131 (1947); (14.5 Mev).

low energy data. The direction of the deviation precludes its explanation as a tensor force effect on the  $P$  waves. Because of the excellent fit to the straight line at lower energies, we find this deviation hard to understand.

### VII. COMPARISON OF PROTON-PROTON AND NEUTRON-PROTON SCATTERING

Breit, Condon, and Present<sup>21</sup> first pointed out the approximate equality of the proton-proton potential and the neutron-proton potential in the singlet state. It is the purpose of this section to compare proton-proton and neutron-proton interactions without calculating the nuclear potential explicitly.

In addition to the functions  $w$ ,  $\varphi$  used in Section V to describe the proton-proton scattering, we shall use also the function  $u$  which would be obtained in the same nuclear potential *without* the Coulomb potential, and its asymptotic function  $\psi$ . Then  $u$  satisfies Eq. (5) and  $\psi$  has the form (7).

The problem is greatly simplified by considering all these functions for energy zero. It is true that direct experiments on proton-proton scattering at this energy would not give any information about the nuclear force between the protons. However, the value of the function  $f$ , Eq. (51) and Fig. 3, for  $E=0$  will give us all the necessary information about the wave functions  $w$  and  $\varphi$  for zero energy, in particular their behavior for small  $r$ . The intercept of the straight line of Fig. 3 gives

$$f(0) = 8.62. \quad (55)$$

We shall first investigate the behavior of the Coulomb comparison function  $\varphi$ . Inserting (51) in (49) we find that for very small  $r$ ,  $\varphi'$  is given by

$$\varphi'_0(r) = (2/D)[\ln(2r/D) + C + \frac{1}{2}f(0)], \quad (56)$$

and that

$$\varphi = 1 + r[\varphi'_0(r) - 2/D]. \quad (56a)$$

In  $\varphi$ , terms of order  $r^2$  have been neglected which will be permissible for our purposes. In  $\varphi'$ , however, we shall need the next term which may be obtained either from YWB or by integration of (39), using (56a):

$$\varphi' = \varphi'_0 + (2r/D)(\varphi'_0 - 4/D). \quad (56b)$$

Now let us obtain a relation between wave functions with and without Coulomb field in the same nuclear potential  $V$  just as we previously compared wave functions of different energy. The wave equations for the two functions to be compared are (37) and (5), and since  $V$  is supposed to be the same, we have, dropping the subscript 1:

$$uw' - wu' \Big|_0^R = (2/D) \int_0^R uwdr/r. \quad (57)$$

A similar relation holds for the "asymptotic func-

tions"  $\psi$  and  $\varphi$  whose wave equations also differ by the Coulomb potential:

$$\psi\varphi' - \varphi\psi' \Big|_{r_1}^R = (2/D) \int_{r_1}^R \psi\varphi dr/r. \quad (57a)$$

In this case, we do not integrate from  $r=0$  because  $\varphi'$  would be infinite at this limit, and the integral on the right-hand side would diverge. We have therefore used an arbitrary lower limit  $r_1$ , and we shall now define  $r_1$  by requiring that the right-hand sides of (57) and (57a) be equal, in other words by the equation

$$\int_{r_1}^{\infty} (\psi\varphi - uw) dr/r = \int_0^{r_1} uw dr/r. \quad (58)$$

An evaluation of  $r_1$  will be given below.

Now, since the right-hand sides of (57) and (57a) have been made equal, the left-hand sides are also equal. At the upper limits, the integrated terms are equal by the definition of  $\psi$ ,  $\varphi$  as the asymptotic expressions for  $u$ ,  $w$ . At the lower limit, the integrated term in (57) is zero, therefore that in (57a) must also be zero. In other words, at the point  $r_1$  the logarithmic derivatives of  $\psi$  and  $\varphi$  are equal,

$$(\psi'/\psi)_{r_1} = (\varphi'/\varphi)_{r_1}. \quad (59)$$

But  $\varphi'/\varphi$  can, at *any* point, be determined from (56a), (56b). On the other hand,  $\psi$  must have the form

$$\psi = 1 - \alpha_P r \quad (60)$$

since it is the asymptotic solution for energy zero in the absence of nuclear and Coulomb potential. The constant  $\alpha_P$  can thus be determined from (59) in terms of the "observed" intercept  $f(0)$ , Eq. (55).

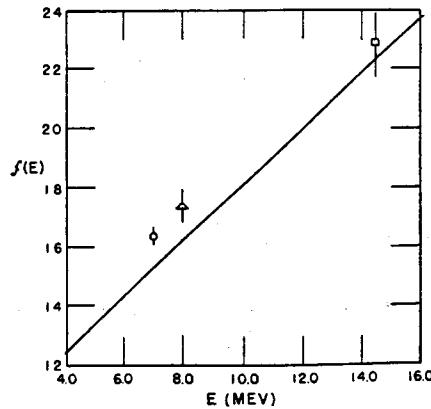


FIG. 4. Experiments on proton-proton scattering from 7 to 15 Mev,  $f$  vs.  $E$ . The straight line is the same as in Fig. 3, the experiments do not agree very well with it.  
 O Dearnley, Oxley, and Perry; Δ Wilson and Creutz;  
 □ Wilson.

Then  $\alpha_P$  can be interpreted as an equivalent reciprocal scattering length, i.e., as the reciprocal scattering length which *would* be obtained for neutron-proton scattering if the nuclear potential were the same as for proton-proton scattering. This can then be compared with the measured  $\alpha_N = 1/a_s$  for singlet neutron-proton scattering.

Inserting (56a), (56b), and (60) into (59) gives, after some simple algebra and neglect of second-order terms in  $r_1/D$ :

$$-\alpha_P = \varphi'_0(r_1) + (4r_1/D)(\varphi'_0 - 2/D), \quad (61)$$

where  $\varphi'_0$  is still given by (56). Greater accuracy could be obtained using the representation of  $\varphi$  in terms of Bessel functions.<sup>20</sup>

That it is possible to find a point  $r_1$  at which the logarithmic slopes of the Coulomb function  $\varphi$  and the straight line  $\psi$  are equal, is due to the peculiar behavior of the Coulomb function (see Fig. 5). As shown by (56a), the function  $\varphi$  begins at  $r=0$  with the value 1 and logarithmically infinite negative slope. It reaches a minimum and then rises. At larger  $r$ , it shows the typical exponential rise expected inside the Coulomb potential barrier. There must therefore be a point where the function  $\varphi$  has the same logarithmic slope as any given straight line.

We shall now determine  $r_1$ . Since  $\varphi'/\varphi$  depends only slightly on  $r_1$  (Eq. (56)), an approximate value of  $r_1$  will be sufficient, and since the Coulomb potential is unimportant inside the nuclear potential, it is permissible to replace the Coulomb functions  $\varphi, \psi$  in the definition (58) of  $r_1$  by the "neutral" functions  $\psi, u$ . We shall do the calculation explicitly for the specially simple case  $\alpha=0$  which

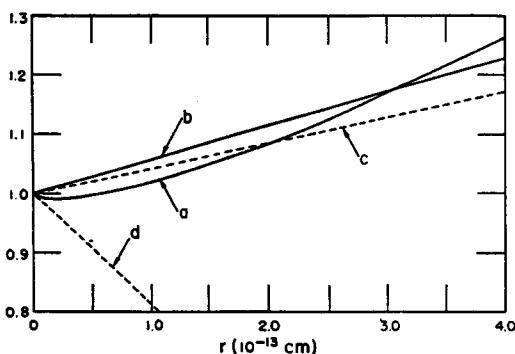


FIG. 5. a) The wave function  $\varphi$  (comparison function) in the Coulomb field, vs. radius, for zero energy with the constant  $\xi$  (Eq. 73a) as given by experiment, b) the function  $\psi$  corresponding to neutron-proton scattering by the same nuclear potential (for a square well), c)  $\psi$  for the actual neutron-proton scattering in the singlet state, d)  $\psi$  for the triplet neutron-proton state. Note the small difference between a, b, and c, the large difference between these and d. Note also the greatly enlarged scale of ordinate: All functions are near unity inside the range of nuclear forces, and b and c agree within a few percent.

corresponds to a resonance level at zero energy. This is a good approximation because  $\alpha$  is actually small; a result for finite  $\alpha$  will be given below. If we take  $\alpha=0$  and a square well,  $u$  is given by  $u_0$  in (35a). Since  $u=\psi$  for  $r>b$ , (58) becomes

$$\int_{r_1}^b \psi^2 dr/r = \ln(b/r_1) = \int_0^b u^2 dr/r = \int_0^b \sin^2(\pi r/2b) dr/r = \frac{1}{2}(C + \ln \pi - Ci\pi), \quad (62)$$

where  $Ci$  is the integral cosine,

$$Ci x = - \int_x^\infty \cos y dy/y. \quad (62a)$$

Therefore

$$\ln(r_1/b) = -0.8245, \quad r_1 = 0.4384b \quad (63)$$

so that  $r_1$  turns out considerably smaller than the effective range which, with our assumptions, is equal to  $b$ . With (54a), we get

$$r_1 = 1.12 \times 10^{-13} \text{ cm}. \quad (63a)$$

We shall show below that (63) remains a very good approximation, even for finite scattering length, but that the approximation would be considerably less good if we replaced  $b$  by  $r_0$  in (63). This makes the calculation slightly involved: one needs  $\alpha$  to obtain  $b$  from  $r_0$  using the curves of BJ, but one needs  $b$  to calculate  $\alpha$ . In practice, a very rough estimate of  $\alpha$  suffices to get an accurate value for  $b$  so that there is no real difficulty.

Using  $b$  from (54a), and using (63), (56), (56a), (61), (38), and (55) we get:

$$\begin{aligned} \varphi_{PS}'(r_1) &= (2/D)[\ln(2b/D) + 4.06] \\ &= 0.568 \times 10^{12} \text{ cm}^{-1}, \end{aligned} \quad (64)$$

$$\varphi_S(r_1) = 1.024, \quad (64a)$$

$$-\alpha_{PS} = 0.585 \times 10^{12} \text{ cm}^{-1}, \quad (65)$$

where the subscripts  $P$  and  $S$  stand for proton and square well, respectively. This result may be compared with the neutron-proton scattering in the singlet state which gives, according to (26a)

$$-\alpha_{NS} = -1/a_{NS} = 0.421 \times 10^{12} \text{ cm}^{-1}. \quad (66)$$

For a Yukawa potential we shall not do the exact calculation but choose an approximate wave function of the form (again for zero binding energy)

$$u_0 = 1 - e^{-\beta r}. \quad (67)$$

As Schwinger<sup>1</sup> has shown, such a wave function when used in the variational method, will give the depth of the potential correctly within 1 part in 10,000. Chew<sup>28</sup> has pointed out that  $u_0$  itself agrees

<sup>28</sup> Geoffrey F. Chew, Phys. Rev. 74, 809 (1948).

## EFFECTIVE RANGE IN NUCLEAR SCATTERING

with the exact wave function within 3 percent. The parameter  $\beta$  is related to the parameter in the meson potential and also directly to the effective range which is

$$r_0 = 2 \int_0^{\infty} (1 - u_0^2) dr = 3/\beta. \quad (67a)$$

For the "effective Coulomb radius" we get then the equation

$$\begin{aligned} \int_{r_1}^R \psi^2 dr / r &= \ln(R/r_1) = \int_0^R u_0^2 dr / r \\ &= \ln(\beta R/2) + C, \end{aligned} \quad (67b)$$

so that

$$\begin{aligned} r_1 &= 2/(\beta\gamma) = 2r_0/3\gamma = 0.374r_0 \\ &= 0.374b = 0.91 \times 10^{-18} \text{ cm}, \end{aligned} \quad (68)$$

using  $b$  from (54b) and with  $\gamma = e^c$ . This gives instead of (64)–(65)

$$\varphi_0 Y' = (2/D)[\ln(2b/D) + 3.90] = 0.509, \quad (69)$$

$$\varphi_Y = 1.014, \quad (69a)$$

$$-\alpha_{PY} = 0.517 \times 10^{12} \text{ cm}^{-1}, \quad (70)$$

where the subscript  $Y$  stands for Yukawa potential.

It is seen that the Yukawa potential gives a result somewhat closer to the neutron-proton result (66). This is in agreement with the result of Breit, Hoisington, Share, and Thaxton<sup>29,4</sup> obtained by explicit calculation of the nuclear potentials. However, the difference between the Yukawa and the square well results is not large, and, judging from Blatt and Jackson's results for other phenomena, the other potentials commonly used (exponential and Gaussian) are almost certain to lie in between. This means, then, that there is a *definite difference* between the nuclear forces in the singlet state for neutron-proton and for proton-proton. This result follows also from the explicit calculations of Breit *et al.*, if the modern value of the neutron-proton cross section, Eq. (20b), is used.

On the other hand, the difference between neutron-proton and proton-proton force is obviously quite small, *viz.* about  $0.1 - 0.16 \times 10^{12} \text{ cm}^{-1}$ . This figure might properly be compared with the reciprocal range of the forces which is about  $4 \times 10^{12} \text{ cm}^{-1}$ . In agreement with this, Breit *et al.*<sup>29</sup> found that the difference between the depths of the two potentials (for the same range and shape) need only be 1.5–3 percent. Thus the hypothesis of the charge-independence of nuclear forces is still very good, provided, of course, that range and shape are the same for which, unfortunately, there is still no experimental proof.

<sup>29</sup> Breit, Hoisington, Share, and Thaxton, Phys. Rev. 55, 1103 (1939).

In (63), (68) we have used wave functions for infinite scattering length. For finite scattering length, the case of a square well can easily be treated and gives

$$r_1 = 0.4384b(1 + 0.114ab + 0.471a^2b^2 + \dots). \quad (71)$$

where  $b$  is the intrinsic range and  $a$  the reciprocal scattering length. Using  $a$  from (65) and  $b$  from (54a), gives for the parenthesis in (71) the value  $1 - 0.0065$ ; an exact calculation gives  $1 - 0.0072$ . Thus  $r_1/b$  is almost unchanged. However,

$$r_0/b \approx 1 - 4\pi^2 ab = 1.0640 \quad (71a)$$

differs appreciably from unity: This shows that it is indeed a much better approximation to use  $b$  in (63) than to use  $r_0$ . Now a slight change in  $r_1$ , by the relative amount  $\epsilon$ , will give a change of  $-\alpha$  by

$$-\delta\alpha = (2\epsilon/D)(1 + 2r_1\varphi_0') = 0.39\epsilon = -0.0028 \quad (71b)$$

with the values of  $\varphi_0'$ ,  $r_1$ , etc. given above. This is practically negligible and changes (65) to

$$-\alpha_{PS} = 0.582 \times 10^{12} \text{ cm}^{-1}. \quad (65a)$$

For the Yukawa well, the approximate wave function

$$u = 1 + ar - e^{-\beta r} \quad (72)$$

gives

$$r_1 = (2/\beta\gamma)[1 - 0.245a/\beta - 0.051a^2/\beta^2 + \dots], \quad (72a)$$

and  $\beta$  is related to the effective range by

$$\beta r_0 = 3 + 4a/\beta. \quad (72b)$$

In our case, we get

$$\begin{aligned} 3r_1\gamma/2r_0 &= 1 - 0.067, \\ b/r_0 &= 1 - 0.097, \\ 3r_1\gamma/2b &= 1.033. \end{aligned} \quad (72c)$$

The change of  $r_1$  with  $a$ , for given  $b$ , is therefore slightly greater than for the square well, and we get

$$\begin{aligned} -\delta\alpha &= 0.0112, \\ -\alpha &= 0.529 \times 10^{12} \text{ cm}^{-1}. \end{aligned} \quad (70a)$$

This makes the difference between Yukawa and square well somewhat smaller, the difference between the proton-proton and neutron-proton scattering somewhat larger.

Finally, we shall compare the asymptotic wave functions with and without Coulomb potential,  $\varphi$  and  $\psi$  (see Fig. 5). The Coulomb function looks fairly complicated, mainly because of its logarithmically infinite slope at  $r = 0$ ; but all this complication makes very little difference for the value of the function, owing to the very large value of the "proton Bohr radius"  $D$  which is about 20 times the effective range. With the constants as observed

(Eq. (55)), the function  $\varphi$  has a minimum at

$$r_{\min} = \frac{1}{2}D e^{-\xi} = 0.216 \times 10^{-13} \text{ cm}, \quad (73)$$

where

$$\xi = C + \frac{1}{2}f(0). \quad (73a)$$

The result (73) is about the Compton wave-length of the proton,  $\hbar/Mc$ . At its minimum,  $\varphi$  has the value

$$\varphi_{\min} = 1 - e^{-\xi} = 0.9925, \quad (73b)$$

which is very close to unity.

The two functions  $\varphi$  and  $\psi$  are very close together for all values of  $r$  inside the range of the nuclear forces. Neglecting higher terms,

$$\psi = 1 + (2r/D)(\xi + \ln 2r_1/D), \quad (74)$$

$$\varphi = 1 + (2r/D)(\xi + \ln 2r/D - 1). \quad (74a)$$

and the ratio is

$$\psi/\varphi = 1 + (2r/D)(\ln r_1/r + 1). \quad (75)$$

As is clear from the definition of  $r_1$  in (59), the ratio

$\psi/\varphi$  has a maximum at  $r=r_1$  whose value is

$$\begin{aligned} \psi(r_1)/\varphi(r_1) &= 1 + 2r_1/D \\ &= 1.040 \text{ for square well} \\ &= 1.032 \text{ for Yukawa potential.} \end{aligned} \quad (75a)$$

At other values of  $r$ , the functions are closer together. This shows that it must be a very good approximation to replace  $\varphi$  and  $w$  by  $\psi$  and  $u$ , respectively, in calculating  $r_1$ . Also it shows that for a given nuclear potential,  $r_0$  and the correction  $P$  (see Section IV) must have substantially the same values as in the absence of the Coulomb potential.

### VIII. ACKNOWLEDGMENTS

I am indebted to Dr. Blatt for valuable discussions, and to him and Mr. Jackson for sending me the manuscript of their paper before publication; it was most valuable to have their numerical results to test and guide the theory. My thanks are also due Dr. Longmire for several calculations, in Sections IV and VI, and for important suggestions (see Section IV).

**Nuclear Many-Body Problem**  
*Phys. Rev.* **103** (5), 1353–1390 (1956)

The aim of this paper is to reconcile the very strong and short range nuclear forces with the shell model in which each nucleon moves in a smooth potential. In addition, my aim was to calculate the characteristics of a heavy nucleus, binding energy and radius, from two-body scattering data; this finally turned out to be impossible. Pandharipande showed that interaction of nucleons by threes must be included.

## Nuclear Many-Body Problem\*

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A self-contained and largely new description is given of Brueckner's method for studying the nucleus as a system of strongly interacting particles. The aim is to develop a method which is applicable to a nucleus of finite size and to present the theory in sufficient detail that there are no ambiguities of interpretation and the nature of the approximations required for actual computation is clear.

It is shown how to construct a model of the nucleus in which each nucleon moves in a self-consistent potential matrix of the form  $\langle \mathbf{r}' | V | \mathbf{r} \rangle$  (Sec. II). The potential is obtained by calculating the reaction matrix for two nucleons in the nucleus from scattering theory. Some complications arise in the definition of the energy levels of excited nucleons (Sec. III). The actual wave function is obtained from the model wave function by an operator which takes into account multiple scattering of the nucleons by each other (Sec. IV).

The method of Brueckner is a vast improvement over the normal Hartree-Fock method since, in calculating the self-consistent potential acting on an individual particle in the model, account is already taken of the correlations between pairs of nucleons which arise from the strong internucleon forces (Sec. V). Although the actual wave function is *derivable* from a wave function which corresponds essentially to the shell model, the probability of finding a large nucleus of mass number  $A$  "actually" in its shell model state is small (of order  $e^{-\alpha A}$ , where  $\alpha$  is a con-

stant) (Sec. VI). The influence of spin is investigated (Sec. VIII). In the case of an infinite nucleus, an integral equation is obtained for the reaction matrix, just as in the theory of Brueckner and Levinson (Sec. IX).

The exclusion principle must be applied in intermediate states in solving the integral equation for the reaction matrix. This makes an enormous difference for the solution. When the exclusion principle is used, the scattering matrix is very nearly given by the Born approximation, for any well-behaved potential (Sec. X). Numerical results are given for the case when nucleons interact only in  $S$  states, an assumption which leads to saturation without a repulsive core. The agreement with observation is fair to poor, owing to the poor assumption for the interaction (Sec. XI). Brueckner's result that three-particle clusters give a small contribution to the energy is confirmed, although the numerical value is many times his result; the calculation is then extended to the case of a repulsive core (Sec. XII). The dependence of the binding energy on the mass number  $A$  is investigated for saturating and nonsaturating interactions (Sec. XIII). Terms of relative order  $1/A$  are calculated, and it is shown that these terms are much smaller than Brueckner and Levinson found, making the method also applicable to relatively small nuclei (Sec. XIV). Some aspects of the problem of the finite nucleus are discussed, including that of degeneracy (Sec. XVI).

## I. INTRODUCTION

**N**EARLY everybody in nuclear physics has marvelled at the success of the shell model. We shall use the expression "shell model" in its most general sense, namely as a scheme in which each nucleon is given its individual quantum state, and the nucleus as a whole is described by a "configuration," i.e., by a set of quantum numbers for the individual nucleons. For instance, the collective model would be included in this definition of the shell model, the only differences being that the potential in which the individual nucleons move is not spherically symmetric but ellipsoidal, and that the emphasis is on different phenomena.

The shell model, defined in this wider sense, has had many triumphs in explaining the positions and properties of states of the nucleus.<sup>1</sup> In addition, Feshbach, Porter, and Weisskopf<sup>2</sup> have shown that the fundamental concept of quantum states of individual nucleons continues to have good meaning even for free neutrons of moderate energy interacting with the nucleus.

While the success of the model has thus been beyond question for many years, a theoretical basis for it has been lacking. Indeed, it is well established that the

forces between two nucleons are of short range, and of very great strength, and possess exchange character and probably repulsive cores. It has been very difficult to see how such forces could lead to any over-all potential and thus to well-defined states for the individual nucleons.

In view of this paradox, it has often been suggested to abandon the idea of interaction of nucleons in pairs inside the nucleus, and to assume instead that nucleons in large aggregates act "collectively" by creating an overall, smoothly varying potential. In particular, it has been suggested<sup>3,4</sup> that there be a general "meson potential" in the nucleus, with high meson density and relatively little variation of the potential from point to point. Such an assumption is again very difficult to reconcile with known facts about mesons: From the analysis<sup>5</sup> of the scattering of mesons of moderate energy (a few hundred Mev), it follows that the coupling of mesons with nucleons is rather *weak* at distances of the order of  $\hbar/\mu c = 1.4 \times 10^{-13}$  cm. Indeed, the coupling at these distances is essentially proportional to the pseudovector coupling constant  $f^2$ , which, according to the analysis<sup>6</sup> of meson scattering, has a value of only about 0.08. The pseudoscalar coupling constant  $g^2 = (2Mf/\mu)^2 \approx 14$  becomes important only for phenomena which involve a transfer of momentum of the order of  $Mc$ , and hence

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<sup>1</sup> M. G. Mayer and J. H. D. Jensen, *Elementary Theory of the Nuclear Shell Model* (John Wiley and Sons, Inc., New York, 1955).

<sup>2</sup> Feshbach, Porter, and Weisskopf, Phys. Rev. 96, 448 (1954).

<sup>3</sup> M. H. Johnson and E. Teller, Phys. Rev. 98, 783 (1955).

<sup>4</sup> L. I. Schiff, Phys. Rev. 84, 1, 10 (1951); 86, 856 (1952).

<sup>5</sup> G. F. Chew and F. E. Low, Phys. Rev. 101, 1570 (1956).

at distances of the order of the proton Compton wavelength  $\hbar/Mc$ . Only at such very small distances from a nucleon will the meson density become high. It is difficult to see how this should lead to a meson potential smooth in space inside the nucleus, or how nonlinear terms in the meson field could be important at an *average* position in the nucleus—of course, they will be very important in the immediate neighborhood of each nucleon. Thus one is automatically led back to the same difficulties which occur when two-body forces between the nucleons are assumed.

But even apart from the specific idea of the meson potential, there are strong arguments to show that the two-body forces continue to exist inside a complex nucleus and are not replaced by a general smooth potential.<sup>6</sup> These arguments have recently been summarized by Brueckner, Eden, and Francis.<sup>7</sup> The point is that there is abundant evidence that the nuclear wave function contains very strong components of high momentum which manifest themselves in such processes as the capture of  $\pi$  mesons and the photoelectric effect caused by high-energy ( $>100$  Mev)  $\gamma$  rays. In both these cases, a large amount of energy without much momentum is given to the nucleus. In order for a nucleon to absorb this energy, and at the same time to conserve momentum, the nucleon must have had a large momentum before it absorbed the  $\pi$  meson or the  $\gamma$  ray; i.e., the wave function of the nucleus in its normal state must contain components corresponding to large momenta of an individual nucleon. Another process in which these components manifest themselves is the “pickup process” in which an incoming proton of high speed picks up a neutron from inside the nucleus to form a deuteron: in order to be “picked up,” the neutron must have had a large momentum in the nucleus. Perhaps the best way of measuring the momentum distribution in the nucleus is to study the energy distribution of protons scattered “quasi-elastically” by a nucleon in the nucleus; this again shows large components at high momentum. All these processes show that the “potential” is fluctuating violently from point to point in the nucleus, which is compatible with the assumption that two-body forces continue to act inside the nucleus without much modification.

Similar difficulties exist in understanding the success of the “cloudy crystal ball” model. It is true that Lane and Wandel<sup>8</sup> could explain that the imaginary part of the potential between nucleon and nucleus is very small, but only by essentially assuming the validity of the shell model. On the other hand, Lane, Thomas, and Wigner,<sup>9</sup> using orthodox methods of quantum mechanics and some seemingly plausible assumptions, obtained

values for this imaginary part which were about 20 times too large. This large result had always been assumed correct before the war, leading to the hypothesis of a “black” nucleus.

Brueckner has developed a powerful mathematical method which for the first time promises to resolve this paradox. In a series of papers with his collaborators, he finds that one can calculate the nuclear energy levels using a self-consistent field method, even though the forces are of short range. Furthermore, the nuclear wave function retains the strong high-momentum components which are indicated by experiment.<sup>7</sup>

The general method has been developed by Brueckner and Levinson,<sup>10</sup> on the basis of the theory of multiple scattering of Watson.<sup>11</sup> The theory was evaluated for a square-well interaction between nucleons by Brueckner<sup>12</sup>; one of his main results was that the nucleons appear to have an effective mass of only about one-half their actual mass; this point will be discussed in Secs. X and XI. Brueckner’s calculation<sup>12</sup> essentially replaced two earlier papers<sup>13</sup> in which a more special assumption was made about the interaction between two nucleons, namely that it was the particular potential derived from meson theory by Brueckner and Watson.<sup>14</sup> The newer approach,<sup>12</sup> in which the nuclear interaction is required only to be in accord with the known facts on two-nucleon scattering and is otherwise left arbitrary, is more satisfactory than the older one,<sup>13</sup> in which the problem of deriving two-body nuclear interactions from meson theory gets mixed up with the entirely separate problem of deriving nuclear structure from a given two-body interaction.

In a further paper,<sup>15</sup> Brueckner finds that for a very large nucleus, the corrections to the self-consistent field approximation are exceedingly small, of the order of 1 part in 1000 of the energy. These corrections arise only from intermediate states in which three (or more) particles are successively excited. In the same paper, Brueckner develops a greatly improved scheme for perturbation theory, the “linked cluster expansion.” Other corrections<sup>16</sup> are of relative order  $1/A$ , where  $A$  is the number of particles in the nucleus (see also Sec. XIV). Further papers have been concerned with applications<sup>16</sup> of the theory and with a different presentation of the method.<sup>17</sup>

In spite of its apparent great accomplishments, the

<sup>10</sup> K. A. Brueckner and C. A. Levinson, Phys. Rev. 97, 1344 (1955). This paper will be quoted as BL.

<sup>11</sup> K. M. Watson, Phys. Rev. 89, 575 (1953); also N. C. Francis and K. M. Watson, Phys. Rev. 92, 291 (1953).

<sup>12</sup> K. A. Brueckner, Phys. Rev. 97, 1353 (1955).

<sup>13</sup> Brueckner, Levinson, and Mahmoud, Phys. Rev. 95, 217 (1954); K. A. Brueckner, Phys. Rev. 96, 508 (1954).

<sup>14</sup> K. A. Brueckner and K. M. Watson, Phys. Rev. 92, 1023 (1953).

<sup>15</sup> K. A. Brueckner, Phys. Rev. 100, 36 (1955). This paper will be quoted as BC.

<sup>16</sup> For example, Brueckner, Eden, and Francis, Phys. Rev. 99, 76 (1955); 100, 891 (1955).

<sup>17</sup> R. J. Eden and N. C. Francis, Phys. Rev. 97, 1366 (1955).

<sup>6</sup> See, e.g., J. Heidmann, Phys. Rev. 80, 171 (1950); J. S. Levinger, Phys. Rev. 84, 43 (1951).

<sup>7</sup> Brueckner, Eden, and Francis, Phys. Rev. 98, 1445 (1955).

<sup>8</sup> A. M. Lane and C. F. Wandel, Phys. Rev. 98, 1524 (1955).

<sup>9</sup> Lane, Thomas, and Wigner, Phys. Rev. 98, 693 (1955).

theory of Brueckner *et al.* has not been readily accepted by nuclear physicists. This is in large measure the result of the very formal nature of the central proof of the theory (reference 10, Sec. II). In addition, the definitions of the various concepts used in the theory are not always clear. Two important concepts in the theory are the wave functions of the individual particles, and the potential  $V$ , "diagonal" in these states (reference 10, Sec. V). The paper by Brueckner and Levinson defines rather clearly how the potential is to be obtained from the wave functions, but not how the wave functions can be constructed from the potential  $V$ . Apparently, BL assume tacitly<sup>18</sup> that the nucleon wave functions are plane waves, but in this case, the method is only applicable to an infinite nucleus. For a finite nucleus, no prescription is given for obtaining the wave functions.

It is the purpose of the present paper to show that the theory of Brueckner gives indeed the foundation of the shell model. It will be shown in Sec. II that a self-consistent scheme *can* be developed for a *finite* nucleus which permits determination not only of its energy levels, but also of the wave functions of the nucleons and of the whole nucleus. This extension, like the original BL scheme, already includes in the self-consistent field all two-particle correlations, which the Hartree method would include in the "configuration interaction" (Sec. V). Essentially, the Hartree method replaces the action of all other particles on a given one by an average potential, while the Brueckner method treats the interaction of any *two* particles exactly, and only replaces the action of any further particles on the interacting pair by an average. Brueckner's method would even give an improvement over the Hartree method for the electrons in an *atom*, and will undoubtedly be very important for the theory of electrons in solids.

In order to satisfy all requirements, the self-consistent potential acting on a nucleon in a finite nucleus must be taken to be a potential matrix,  $(\mathbf{r}'|V|\mathbf{r})$ , or transformed to momentum space,  $(\mathbf{k}'|V|\mathbf{k})$ . The Hartree method which uses a potential  $V(\mathbf{r})$ , and the original BL method for an infinite nucleus which gives a potential  $V(\mathbf{k})$  depending on momentum only, are then special limits of our self-consistent potential.

An actual solution of the problem is attempted only for an infinite nucleus. In this case, the choice of wave functions is obvious, namely plane waves. Then the problem reduces to the determination of the reaction matrix of scattering theory for a given set of nucleon wave functions. This requires the solution of an integral equation in momentum space (Sec. IX). From the derivation of this equation, it is clear that the intermediate states must satisfy the exclusion principle; this fact was realized by Brueckner, but was not taken into

account in his actual solution. In fact, the exclusion principle is found to have a decisive influence on the solution (Sec. X). Fortunately, the exclusion principle makes the integral equation *easier* to solve, by virtue of the rather large radius of the Fermi sphere of occupied states in momentum space. If the potential is well-behaved, in particular if it does not contain a repulsive core, the scattering matrix turns out to be essentially equal to the matrix of the interaction potential between two nucleons. This result, which would not be true without the exclusion principle, means, most surprisingly, that the theory reduces nearly to the Born approximation. The error in the Born approximation is only about 5%.

This result is closely connected with the rapid convergence of the theory itself. Brueckner<sup>15</sup> already realized that the correction terms due to three-particle clusters (and higher order perturbations) are small only by virtue of the Pauli principle. Our own recalculation of the three-particle cluster correction gives a result about 20 times larger than Brueckner's (Sec. XII) but still small enough to guarantee rapid convergence of the theory, *i.e.*, about 1% of the main term in the interaction. The successive approximations are then (1) the Born approximation, (2) the correction arising from the solution of the two-particle scattering equation which is about 5% of the first approximation, (3) the three-particle cluster term which is about 1% of the first order. Thus the successive approximations converge by about equal steps, which is very plausible. (In Brueckner's original theory, the second approximation was about equal to the first and the third only about 0.1 percent of it, which seemed rather miraculous.) Indeed, once the importance of the Pauli principle is realized, it would seem possible—for a well-behaved nuclear interaction—to solve the entire nuclear problem by a suitably arranged perturbation theory.

This is not possible, of course, if the interaction between nucleons contains a repulsive core. In this case, the Born approximation would give an infinite result, and the reaction matrix is in no way similar to the Born approximation. To include the Pauli principle in this case, a different treatment is required; this will be discussed in a future paper by Bethe and Goldstone. The exclusion principle can be shown to act like an increase of the effective radius of the core.

In order to obtain a feeling about the orders of magnitude, a special model is calculated in Sec. XI. Since the results on repulsive-core potentials are not yet available, a different potential was postulated which would give nuclear saturation in a simple way. Interaction was assumed to exist only in  $s$  states, as Brueckner<sup>12</sup> did in his evaluation. The results are fair to poor; in particular, the equilibrium density comes out about 30 times too high. This is not too surprising in view of the arbitrary nature of the potential assumed.

Indeed, we consider it premature to attempt to

<sup>18</sup> This assumption is only mentioned once in their paper, and this as late as Sec. VI.

obtain quantitative results from the Brueckner method until the method itself is fully established, including a treatment of a repulsive core plus an attractive potential together with the Pauli principle. Once the method is established, there will still remain the question of the proper two-nucleon potential to be used. It is not at all likely that all potentials which give the same nucleon-nucleon scattering at low energy, will also give the same nuclear binding energies; in fact, the example of the repulsive core shows that this cannot be generally the case. It will be very interesting to see whether we can learn additional facts about the nucleon-nucleon interaction from a study of complex nuclei.

In any case, confidence in the Brueckner method cannot be based on numerical agreement (or lack of agreement) between the results derived from it and experiment. Such agreement will show whether the assumptions made about nuclear forces are acceptable or not. The *method* must rest entirely on mathematical proof and internal consistency.

Some contributions are made in this paper towards the mathematical development. In Sec. III, the steps required to obtain the reaction matrix are discussed explicitly. Certain complications appear; in particular, it is not possible to assign a unique energy to a nucleon in an excited state. Fortunately, these problems are of no practical importance for well-behaved potentials. In Sec. IV, the model operator connecting the actual wave function with the model wave function, is written down. In Sec. VII, the definitions are discussed which are necessary to make the theory applicable to finite nuclei. In Sec. VIII, the influence of nucleon spin and charge, and their behavior in intermediate states, are treated in detail.

Brueckner and Levinson<sup>10</sup> have shown that there are certain correction terms in the theory which are of order  $1/A$ . In Sec. XIV it is shown that these are numerically about 100 times smaller than BL found, i.e., they are of the order of  $1/A$  times the three-particle cluster corrections of Sec. XII. Matrix elements, which correspond to the excitation of one nucleon rather than two, and which would vanish for an infinite nucleus, likewise give contributions of order  $1/A$  or less (Sec. XV).

Brueckner<sup>11</sup> has obtained the somewhat surprising result that the energy of any large system should be proportional to the number of particles,  $A$ . It is pointed out that this holds only if the density is kept fixed. The actual energy is obtained by varying the density until the energy is a minimum; then only saturating forces give an energy proportional to  $A$  for the system; for nonsaturating systems for which the density varies with  $A$ , the energy per particle also varies (Sec. XIII).

The problems for finite nuclei are discussed in Sec. XVI. They are essentially two, *viz.* (a) the behavior of the self-consistent potential near the surface of the nucleus and (b) the degeneracy of many configurations.

Configuration interaction should be taken into account only between degenerate configurations. The theory has enough flexibility to permit a definition of "degeneracy" which is convenient for calculation. Generally, the theory justifies in all essential respects the practice of current shell model calculations.

The reader who is interested in results but not in complicated theoretical developments, is advised to read Sec. II, then Eq. (3.1) and the explanation of the symbols in it but not the rest of Sec. III, then Secs. IX-XII and XVI. The other sections may be left out without essential loss of continuity. A knowledge of the papers by Brueckner and collaborators<sup>10-17</sup> is not required.

## II. DEFINITION OF SELF-CONSISTENT FIELD

We consider a finite (but large) nucleus. We shall assume a potential  $V$  in which each individual nucleon moves, then calculate the wave functions of the nucleons in this potential, and then construct the potential  $V$  again from the wave functions. The resulting potential should of course be equal to the starting potential—this is the condition of self-consistency.

The potential  $V$  must be assumed to be a potential matrix,

$$\langle \mathbf{r}' | V | \mathbf{r} \rangle, \quad (2.1)$$

rather than a simple potential such as is assumed in the Hartree theory for atoms. In that theory, it is assumed that

$$\langle \mathbf{r}' | V | \mathbf{r} \rangle = V(\mathbf{r})\delta(\mathbf{r}' - \mathbf{r}). \quad (2.2)$$

That the more general assumption (2.1) is necessary, follows from Brueckner's<sup>12</sup> result for the infinite nucleus, *viz.*, that the diagonal elements of  $V$  in a momentum representation depend strongly on the momentum  $\mathbf{k}$  (see also Secs. X and XVI of this paper). Such velocity-dependent potentials can, in ordinary space, be represented only by a nonlocal potential matrix (2.1). This generalization of the potential concept is one of the reasons why Brueckner's method has so much greater power than the original Hartree method. In effect, a nonlocal potential (but of course one of special type) is already used in the Fock method.

A state of a nucleon in the potential (2.1) must satisfy the Schrödinger equation ( $\hbar=1$ ):

$$(1/2M)\nabla^2\psi_n(\mathbf{r}) + E_n\psi_n(\mathbf{r}) = \int d^3\mathbf{r}' \langle \mathbf{r}' | V | \mathbf{r} \rangle \psi_n(\mathbf{r}'). \quad (2.3)$$

The  $\psi_n$  form a complete set, and can easily be shown to be orthogonal:

$$\int \psi_{n'}^*(\mathbf{r})\psi_n(\mathbf{r})d^3\mathbf{r} = 0, \quad \text{if } E_n \neq E_{n'}. \quad (2.4)$$

For reasonable assumptions about the potential, i.e., essentially a well of a certain radius, there will be discrete states (the states of the shell model) for  $E_n < 0$ , and continuum states for  $E_n > 0$ .

A state of the nucleus is defined by specifying which of the one-nucleon states  $\psi_n$  are occupied by nucleons. The set of occupied one-nucleon quantum states will be called the "configuration." Each configuration will be described by a Slater determinant wave function which contains all the occupied one-nucleon states. This determinant we call the model wave function and we denote it by  $\Phi$ . Because of the properties of the nucleon wave functions, the model wave functions for different configurations are orthogonal. It is essential for this purpose that all nucleon wave functions are taken in the same potential  $V$ . For the present we disregard degeneracies (see, however, Sec. XVI).

Among the configurations, we single out one whose properties we wish to calculate. This we call the chosen configuration. This need not necessarily be the lowest state of the nucleus, but we shall generally consider states of relatively low energy (say, below 20-Mev excitation energy). Throughout this paper, the properties of this chosen configuration will be calculated more carefully than those of other configurations.

It is often convenient to assign definite quantum numbers to each nucleon, e.g., by considering the main diagonal of the Slater determinant. Thus we may speak of the state  $n_i$  of nucleon  $j$ ; the states in the chosen configuration we shall denote by superscripts 0, thus:  $n_i^0$ .

Now the actual interaction between two nucleons is introduced; following Brueckner, it will be denoted by  $v$ . It is a function of the distance between the two nucleons,  $r_{ij}$ , their spins and charge, and it may contain exchange operators. It is assumed to be determined from experiments on the two-nucleon system. Three-body forces are assumed to be negligible. Whether this is in fact true for nuclear forces is not known at present; but it is clearly the simplest assumption to make, at least until it is clearly proved that no agreement with observation can be obtained without three-body forces.

The matrix elements of the known operator  $v_{ij}$  can be determined between two arbitrary configurations of nucleons. Obviously, the states of all nucleons other than  $i$  and  $j$  must remain unchanged in the transitions. The states of all these other nucleons will influence the matrix elements of  $v_{ij}$  only indirectly, by determining the potential operator  $(\mathbf{r}'|V|\mathbf{r})$  of the self-consistent field and thereby the wave functions  $\psi_i$  and  $\psi_j$ . However, since we now consider the wave functions  $\psi_n$  in the potential  $V$  as given, we need only consider matrix elements such as

$$(n_i' n_j' | v_{ij} | n_i n_j)_N, \quad (2.5)$$

where the subscript  $N$  indicates that the matrix element is to be taken between the determinant (model) wave functions describing the initial and final configurations of the nucleus, which contain nucleons  $i$  and  $j$  in the states  $n_i$ ,  $n_j$  and  $n_i'$ ,  $n_j'$ , respectively. We shall assume that all other nucleons are in the states prescribed by

the chosen configuration,  $n_k^0$ . The states  $n_i$ ,  $n_j$ ,  $n_i'$ ,  $n_j'$  need not coincide with  $n_i^0$  and  $n_j^0$ , respectively.

The matrix element (2.5) vanishes automatically if any one of the four states  $n_i$ ,  $n_j$ ,  $n_i'$  or  $n_j'$  coincides with one of the states occupied by one of the other nucleons,  $n_k^0$ , or if  $n_i = n_k^0$  or  $n_i' = n_k^0$ . If none of these prohibitions due to the Pauli principle exists, we have

$$(n_i' n_j' | v_{ij} | n_i n_j)_N = (n_i' n_j' | v_{ij} | n_i n_j)_P - (n_i' n_i' | v_{ij} | n_i n_j)_P, \quad (2.6)$$

where the matrix elements with the subscripts  $P$  are taken without regard to the presence of other nucleons, and are given by

$$(n_i' n_j' | v_{ij} | n_i n_j)_P = \int \psi_{n_i}^*(\mathbf{r}_i) \psi_{n_j}^*(\mathbf{r}_j) v_{ij}(\mathbf{r}_{ij}) \times \psi_{n_i}(\mathbf{r}_i) \psi_{n_j}(\mathbf{r}_j) d^3 r_i d^3 r_j. \quad (2.7)$$

The integrals in (2.7) imply also summations over spin and charge, and the operator  $v_{ij}$  may involve spin and charge operators. The second term in (2.6) is the well-known exchange term. There are obvious selection rules between primed and unprimed nucleon states.

It will be useful to consider a very large nucleus. Then the wave functions over most of the nucleus can be approximated by plane waves. This model will be used predominantly from Sec. IX on. In this case, momentum will be conserved between the two nucleons, viz.,

$$\mathbf{k}_i' + \mathbf{k}_j' = \mathbf{k}_i + \mathbf{k}_j. \quad (2.8)$$

Then the final spatial wave function of nucleon  $j$  is completely specified if that of nucleon  $i$ , and the initial states of both, are given.

In the next section, we shall show how at least the most important matrix elements of  $V$ , the one-nucleon potential, can be determined from the interaction  $v_{ij}$ . These matrix elements are obtained with respect to the wave functions  $\psi_n(\mathbf{r})$  ( $n$  representation). Once they are known, we may obtain  $V$  in the  $\mathbf{r}$  representation by the usual formula of transformation theory:

$$(\mathbf{r}'|V|\mathbf{r}) = \sum_n \sum_{n'} \psi_n^*(\mathbf{r}') (n'|V|n) \psi_{n'}(\mathbf{r}). \quad (2.9)$$

For self-consistency, the resulting  $(\mathbf{r}'|V|\mathbf{r})$  must be identical with the initial  $V$  used in Eq. (2.3). Just as in the original Hartree theory, this self-consistency must be achieved by trial and error.

BL developed their theory without first defining a potential  $V$ . This was made possible by their tacit assumption<sup>18</sup> that the one-nucleon wave functions are plane waves. This assumption is appropriate for an infinite nucleus and follows in this case from the general argument of invariance of all physical quantities with respect to translation. Thus in this special case a knowledge of the potential  $V$  is not required to obtain the wave functions. In the case of a finite nucleus, just as in the case of the Hartree-Fock atom, the first step in the development of the self-consistent

field must be a "guess" of the one-particle potential  $V$ . Our method in this paper contains the Hartree-Fock theory as an approximation (Sec. V) and goes over into the Brueckner-Levinson theory in the limit of an infinite nucleus (Sec. IX).

In every case, and thus also in the case of an infinite nucleus, the set of one-nucleon wave functions must be uniquely defined. The fact that the wave functions in an infinite nucleus must be plane waves defines them except for one parameter, *viz.*, the density of the nucleus. To determine the density, the self-consistency requirement must be used. Eden<sup>19,20</sup> has shown that this requirement can be satisfied by formally calculating the energy of the nucleus as a function of the density, and then finding the minimum of this function. Thus the self-consistency in this case is equivalent to the variational problem. This will be discussed in more detail in Sec. IX, and also in E,<sup>20</sup> Sec. IV.

### III. REACTION MATRIX

The main feature of the Brueckner theory is the use of the reaction matrix<sup>21</sup> for the scattering of two nucleons while they are moving in the nuclear medium. Consider, for example, the scattering of two nucleons  $i$  and  $j$  from their states  $n_i^0, n_j^0$  in the chosen configuration to some other states  $n_i', n_j'$ . The reaction matrix  $G$  for this problem is the solution of the equation:

$$(n_i', n_j' | G_{ij} | n_i^0 n_j^0) = (n_i' n_j' | v_{ij} | n_i^0 n_j^0) + \sum_{n_i'' n_j''} (n_i' n_j' | v_{ij} | n_i'' n_j'')_N \times \frac{Q}{(n_i'' n_j'' | G_{ij} | n_i^0 n_j^0)}. \quad (3.1)$$

The denominator  $e$ , or rather  $-e$ , means the excitation energy of the two nucleons  $i$  and  $j$  in the intermediate state  $n_i'' n_j''$ , as compared with their state  $n_i^0 n_j^0$  in the chosen configuration, both calculated in the nuclear medium, i.e., under the influence of all the other nucleons. It will be calculated presently.

It is clearly necessary to exclude states for which  $e=0$ . This is done by BL by using the principal value in their Eq. (3) which corresponds to our (3.1). (Since they are dealing with an infinite nucleus their Eq. (3)

contains an integral over intermediate states rather than a sum.) Following Eden,<sup>20</sup> we have introduced the operator  $Q$  to fulfill the same purpose as the principal value operator: we define  $Q$  to be zero for all states for which  $e=0$ , i.e., for the chosen configuration and for all other configurations which have the same energy. In addition, we are free to set  $Q=0$  for all configurations which have nearly the same energy as the chosen one, as long as we specify clearly at the beginning of any particular calculation which configurations we shall thus regard as "nearly degenerate." This will be discussed further in Sec. XVI, where it will be explained why this freedom in the definition of  $Q$  is useful.

It may be noted in passing that singly excited states cannot be reached from the chosen configuration in the case of an infinite nucleus because of the momentum conservation (2.8); i.e., for an infinite nucleus it is impossible to excite one nucleon without also exciting the other. In a large but finite nucleus, the matrix elements  $(n_i^0 n_j'' | v_{ij} | n_i^0 n_j^0)$  are not zero but small, of order  $\Omega^{-1}$  (where  $\Omega$  is the volume of the nucleus) compared with those elements in which both nucleons are simultaneously excited with (approximate) momentum conservation (see Sec. XV); leaving them out in (3.1) would therefore be no great change and will be done at various points to simplify the calculation.

As has been pointed out in Sec. II, the matrix elements  $v_N$  of the interaction between states of the complete nucleus vanish if any of the states  $n_i^0 n_j'' n_k^0$  is occupied by some other nucleon  $k \neq i, j$  in the chosen configuration, i.e., if any of them is equal to some  $n_k^0$ . Thus either these states  $n_i'$ , etc. are the states of nucleons  $i$  and  $j$  themselves in the chosen configuration, i.e., they are  $n_i^0$  and  $n_j^0$ , or they must be outside the chosen configuration, i.e., they are normally unoccupied states. For the final state  $n_i' n_j'$ , both of these possibilities exist. For the intermediate state  $n_i'' n_j''$ , however, the operator  $Q_{ij}$  (as defined) excludes the possibility that either  $n_i''$  or  $n_j''$  is equal to the chosen states  $n_i^0, n_j^0$ : therefore, in this case, both nucleons must be in normally unoccupied states. Thus the Pauli principle must operate in the intermediate state. We could indicate this by explicitly summing in (3.1) only over unoccupied states  $n_i''$  and  $n_j''$ .

The Pauli principle has the consequence that the denominators  $e$  are in general not even nearly zero, especially if the ground state of the nucleus is calculated. The  $e$  are all negative. Further, the matrix  $G_{ij}$  has by (3.1) the same selection rules as  $v_{ij}$ : it vanishes if  $n_i'=n_j'$ , or if either  $n_i'$  or  $n_j'$  is equal to any of the states occupied by other nucleons,  $n_k^0$ . In this way, the matrix  $G_{ij}$  depends on the entire chosen configuration and not merely on the states of nucleons  $i$  and  $j$ .

The excitation energy  $-e$  is given by

$$-e = E(B) - E(C), \quad (3.2)$$

where  $E(C)$  is the energy of the chosen configuration  $C$ , and the intermediate configuration  $B(n_i' n_j')$  differs

<sup>19</sup> R. J. Eden, Phys. Rev. 99, 1418 (1955).

<sup>20</sup> R. J. Eden, Proc. Roy. Soc. (London) A235, 408 (1956). This paper will be quoted as E.

<sup>21</sup> The real solution of the scattering equation (3.1), corresponding to standing waves, is required, not the complex solution corresponding to outgoing waves; therefore we are dealing with a reaction rather than a scattering matrix. Accordingly, the notation  $G_{ij}$  is not appropriate since it is commonly used for the complex scattering matrix. We did not wish to use  $r$  or  $R$  because the distance between nucleons and the nuclear radius occur frequently, and we have therefore adopted the notation  $G$  used by M. L. Goldberger, Phys. Rev. 84, 929 (1951). Avoidance of  $i$  also has the advantage of making the notation more different from that for the kinetic energy for which we use  $T$ , as Eden does in E. We think that  $H_0$  for the kinetic energy should be avoided since the free-nucleon assumption does not afford even a "zero-order" approximation to the problem.

from  $C(n_i^0 n_j^0)$  by having the states  $n_i^0$  and  $n_j^0$  empty and the states  $n_i$  and  $n_j$  filled. It will be shown in Sec. IV, after Eq. (4.17), that for any configuration with states  $n_i$  occupied, one has in good approximation

$$E = \sum_i (n_i | T_i | n_i) + \sum_{ij} (n_i n_j | G_{ij} | n_i n_j) + w_{1c}, \quad (3.3)$$

where  $w_{1c}$  is a constant which is nearly the same for all states of low excitation, and which therefore cancels in taking the difference (3.2). Now the interactions  $G_{kl}$  between any two nucleons  $k, l$  other than  $i, j$  are the same in the two configurations  $B$  and  $C$  and therefore cancel in (3.2). Therefore we get

$$-e_{ij} = E(n_i, n_j; n_i^0, n_j^0) + \Delta G_{ij}, \quad (3.4)$$

where

$$\begin{aligned} & \mathcal{E}(n_i, n_j; n_i^0, n_j^0) \\ &= (n_i | T_i | n_i) + \sum_{k \neq i} (n_i n_k^0 | G_{ik} | n_i n_k^0; n_i^0 n_j^0, n_j) \\ &\quad - (n_i^0 | T_i | n_i^0) - \sum_{k \neq i} (n_i^0 n_k^0 | G_{ik} | n_i^0 n_k^0) \\ &\quad + \text{same for nucleon } j \quad (3.5) \end{aligned}$$

may be considered as the excitation energy of nucleons  $i$  and  $j$  in the field of all the others.

The quantum numbers listed after the semicolon in the first  $G_{ik}$  matrix in (3.5) give the empty states and the extra occupied state in configuration  $B$ . The last term in (3.4) is

$$\begin{aligned} \Delta G_{ij} &= (n_i n_j | G_{ij} | n_i n_j) - (n_i n_j^0 | G_{ij} | n_i n_j^0) \\ &\quad - (n_i^0 n_j | G_{ij} | n_i^0 n_j) + (n_i^0 n_j^0 | G_{ij} | n_i^0 n_j^0). \quad (3.6) \end{aligned}$$

Since this is only the interaction between one pair of nucleons while (3.5) is the interaction between one nucleon and  $A$  others,  $\Delta G_{ij}$  is of relative order  $1/A$ . We shall therefore neglect it although it could be taken into account if we desired.

The reaction matrix  $(n_i n_k^0 | G_{ik} | n_i n_k^0; n_i^0 n_j^0, n_j)$  is calculated by solving an equation similar to (3.1). However, we must remember that in configuration  $B$  the states  $n_i^0$  and  $n_j^0$  are empty, whereas there is an extra nucleon in state  $n_j$ . Therefore we must count the excitation energy of nucleon  $i$  from the empty state  $n_i^0$ , not from the "initial" state  $n_i$ . Further, we must include in the energy denominator the constant excitation energy of nucleon  $j$  in going from state  $n_j^0$  to  $n_j$ . Explicitly, we have to solve

$$\begin{aligned} & (n_i' n_k' | G_{ik} | n_i n_k^0; n_i^0 n_j^0, n_j) \\ &= (n_i' n_k' | v_{ik} | n_i n_k^0)_N - \sum (n_i' n_k' | v_{ik} | n_i'' n_k'') \\ &\quad \times \frac{Q_a}{\mathcal{E}(n_i'', n_j, n_k''; n_i^0 n_j^0, n_k)} \\ &\quad \times (n_i'' n_k'' | G_{ik} | n_i n_k^0; n_i^0 n_j^0, n_j). \quad (3.7) \end{aligned}$$

The denominator  $\mathcal{E}(n_i'', n_j, n_k''; n_i^0 n_j^0, n_k)$  is a sum of three terms similar to the two in (3.5). Thus it is

ordinarily "larger" than the denominator (3.5) occurring in (3.1). This effect has been mentioned by Brueckner<sup>16</sup> in BC and called "propagation off the energy shell." In a naive application of the theory of the scattering matrix, one might have expected the denominator  $\mathcal{E}(n_i', n_k'; n_i, n_k)$  instead of that found in (3.7); this would be much smaller and might even become zero or negative.

The excitation energy (3.5) can in general not be written as

$$\mathcal{E}(n_i, n_j; n_i^0, n_j^0) = E(n_i) + E(n_j) - E(n_i^0) - E(n_j^0), \quad (3.8)$$

i.e., as the difference between the energies of particles  $i$  and  $j$  in the now occupied state and in the chosen state. It is true that the second line of (3.5) may be considered as the energy of particle  $i$  in the chosen configuration,

$$E(n_i^0) = (n_i^0 | T_i | n_i^0) + \sum_{k \neq i} (n_i^0 n_k^0 | G_{ik} | n_i^0 n_k^0). \quad (3.9)$$

But the first line of (3.5) depends not only on the state occupied by particle  $i$  in configuration  $B$ , but also on the two empty states  $n_i^0, n_j^0$  and on the state  $n_j$  now occupied by particle  $j$ ; it can therefore not be written as  $E(n_i)$ . We cannot define the energy of a normally empty state  $n_i$ , but this energy depends on the other states which are empty or occupied.<sup>22</sup> The energy " $E(n_i) + E(n_j)$ " depends not just on two labels,  $n_i, n_j$ , but on four,  $n_i, n_j, n_i^0$  and  $n_j^0$ .

This is obviously a rather complicated situation. Fortunately, for the two most important types of interaction the dependence on all the additional quantum numbers is not great, so that (3.8) is probably a good approximation. The first type is a simple interaction of the "classical" type, like Yukawa, square well, etc., without a repulsive core. For this type, it will be shown in Sec. X that the sum term on the right-hand side of (3.1) or (3.7) gives a relatively small contribution, so that for instance (3.7) reduces nearly to the first term on the right, the interaction matrix  $v_{ik}$ . This then does not depend on the supernumerary quantum numbers  $n_i^0, n_j^0, n_k$ , and in this case the first line of (3.5) is a function of  $n_i$  alone so that (3.8) is valid.

The second important type of interaction is a repulsive core.<sup>23</sup> In this case the difference between the interaction matrix  $v$  and the reaction matrix  $G$  is large. However, the main contribution to the sum in (3.1) comes from intermediate states of very high energy. For these states, the kinetic energy term  $(n_i | T_i | n_i)$  in (3.5) is far more important than the interaction term  $G$ . This kinetic energy, however, depends only on the state  $n_i$ , not on  $n_i^0, n_j^0$ , and  $n_j$ .

We shall therefore assume in most of our calculations

<sup>16</sup>I am indebted to J. Goldstone for pointing this fact out to me.

<sup>22</sup>This interaction will be treated in a forthcoming paper by the author and J. Goldstone, to be published in Proc. Roy. Soc. (London), which will be quoted as BG.

that (3.8) is a good approximation. It is, however, an approximation only; in BL and other papers of the Brueckner school, it was assumed to be exact, and it was assumed to be the only task of the theory to determine the dependence of the eigenvalue  $E(n)$  on the momentum  $k$ . The difficulty of defining  $E(n)$  for unoccupied states  $n$  exists whether we treat an infinite nucleus or a finite one.

However, for a finite nucleus the difficulty has a further unpleasant consequence: it makes it impossible to give a unique definition of the one-particle potential  $V$ . It would obviously be desirable to define  $V$  in such a way that the excitation energy of a particle as defined by (3.5), agrees with the difference of the eigenvalues of the particle calculated by solving (2.3) in the given potential  $V$ . But this cannot be done since the excitation energy (3.5) can in general not be written in the form (3.8). Therefore (3.5) cannot be simplified by introducing one-particle eigenvalues.

It is possible, however, to define  $V$  in such a way that the eigenvalue  $E(n_i^0)$  represents the energy required to remove particle  $i$  from the chosen configuration. This energy is given by the second line of (3.5). Thus we wish to choose  $V$  in such a way that

$$(n_i^0 | V | n_i^0) = \sum_{k \neq i} (n_i^0 n_k^0 | G_{ik} | n_i^0 n_k^0) \quad (3.10)$$

for all states  $n_i^0$  in the chosen configuration. The  $G_{ik}$  in (3.10) do not depend on any quantum numbers except  $n_i^0$  and  $n_k^0$ , in contrast to the  $G_{ik}$  occurring in (3.7). The right-hand side of (3.10) therefore depends only on  $n_i^0$ , once the chosen configuration is selected. By the way, the sum on the right-hand side of (3.10) may be extended to include  $k=i$  because this term is automatically zero owing to the Pauli principle. The eigenvalue of a nucleon in an occupied state of the chosen configuration is then

$$E(n) = (n | T | n) + \sum_j (nn_j^0 | G | nn_j^0). \quad (3.11)$$

It is also possible to define uniquely the elements of  $V$  leading from an occupied to an empty state, by setting

$$(n_i | V | n_i^0) = \sum_j (n_i n_j^0 | G_{ij} | n_i^0 n_j^0), \quad (3.12)$$

where again the term  $j=i$  gives zero contribution. In the final state, only the state  $n_i^0$  of the chosen configuration is empty and  $n_i$  outside that configuration is occupied; thus the matrix element depends on these two quantum numbers.

However, it is not possible to give any unique definition of the elements of  $V$  between two *unoccupied* states, diagonal or nondiagonal. The diagonal elements should be given by the second term on the right of (3.5),

$$(n_i | V | n_i) = \sum_{k \neq i} (n_i n_k^0 | G_{ik} | n_i n_k^0; n_i^0 n_k^0, n_i), \quad (3.13)$$

but as we have seen, they depend not only on the state of the nucleon  $n_i$  considered, but also on the states  $n_i^0$ ,

$n_i^0$ , and  $n_j$ . If  $(n_i | V | n_i)$  for an unoccupied state  $n_i$  must be defined, one might take a suitable average of (3.13) over  $n_i^0$ ,  $n_j^0$ , and  $n_j$ . This obviously would have no physical meaning, but would serve merely to give a definition of the self-consistent potential  $(r' | V | r)$ . To obtain this potential from (2.9), all matrix elements  $(n' | V | n)$  must be known.

As we have seen, the matrix elements starting from occupied states are well defined. The nondiagonal matrix elements  $n' \neq n$  are small, of order  $\Omega^{-1}$  if the nuclear volume  $\Omega$  is large (Sec. XV). The diagonal elements,  $n' = n$  (unoccupied), can only be defined with some arbitrariness. To see what this arbitrariness means for the potential  $(r' | V | r)$ , let us assume that we can use plane wave functions, which is legitimate for a large nucleus. Then the contribution of the diagonal elements for unoccupied states to (2.9) is

$$\begin{aligned} \sum_{n(\text{unocc.})} \psi_n^*(r') (n | V | n) \psi_n(r) \\ = (2\pi)^{-1} \int_{kp}^{\infty} dk (k | V | k) e^{ik \cdot (r-r')}. \end{aligned} \quad (3.14)$$

This is therefore associated with the behavior of  $(r' | V | r)$  as a function of  $r - r'$ , and particularly with the rapid oscillations of this function. Presumably, these have little influence on the wave functions  $\psi_n$  which are solutions of the Schrödinger equation in this potential. For a large nucleus, these wave functions are essentially free-particle functions in a box. Therefore we believe that the arbitrariness in the matrix elements of  $V$  between unoccupied states will not have very much influence on the set of wave functions  $\psi_n$  for the individual nucleons.

The following may be an acceptable procedure: choose  $(r' | V | r)$  by "guessing," and calculate the  $\psi_n$ , the interaction matrix  $v_{ij}$ , and the reaction matrix  $G_{ij}$ . Then calculate the matrix elements of  $V$  between *occupied* states from (3.11) and (3.12); they are well defined. If they do not agree with the corresponding matrix elements of the originally chosen  $(r' | V | r)$ , correct the latter suitably. However, do not attempt to correct or even define the matrix elements of  $V$  between unoccupied states, but instead rely on the "first guess" of  $V$  in this respect. This would presumably simplify the procedure of obtaining a self-consistent solution.

It is essential that  $V$  be the same potential for all states  $\psi_n$  of single nucleons, in order to guarantee orthogonality.

#### IV. CONCERNING THE PROOF OF THE METHOD

Following BL,<sup>10</sup> the actual wave function  $\Psi$  of the nucleus in any given configuration (not necessarily the ground state) is related to the model wave function by an operator  $F$ , thus

$$\Psi = F\Psi. \quad (4.1)$$

$F$  has been called the model operator by Eden,<sup>20</sup> and it is defined implicitly by the two equations

$$F = 1 + \frac{Q}{e} \sum_{ij} I_{ij} F_{ij}, \quad (4.2)$$

$$F_{ij} = 1 + \frac{Q}{e} \sum_{lm \neq ij} I_{lm} F_{lm}, \quad (4.3)$$

where the sums go over all pairs of nucleons, each pair being counted only once, and the second sum excludes the term in which both nucleons  $l$  and  $m$  are identical with the nucleons  $i$  and  $j$ , but includes terms in which *one* of the two nucleons  $l, m$  coincides with one of the pair  $i, j$ . The operator  $I$  is related to the scattering matrix  $G$  defined in Sec. III. We write

$$I_{ij} = G_{ij} - \tilde{G}_{ij}, \quad (4.4)$$

and, following Eden, we define  $\tilde{G}_{ij}$  as the operator which comprises the diagonal elements of  $G_{ij}$  and those in which the state of only *one* nucleon changes; for a more precise definition, see Sec. VII and E. Then  $I_{ij}$  is essentially the "nondiagonal" part of the operator  $G_{ij}$ , more precisely the part which corresponds to the simultaneous change of the quantum states of both nucleons  $i$  and  $j$ . "Diagonal" is to be understood with respect to the set of model wave functions defined in Sec. II. The denominators  $-e$  denote the excitation energy of the nucleus in the model state which is established when the operators to the right of  $e$  have operated on the "initial" model wave function  $\Phi$  of Eq. (4.1).

The excitation energy is to be calculated as in (3.4), by taking the difference of the *model* energies between the excited and the chosen configuration [see Eq. (4.19)]. One must not use the difference between the actual energies, and certainly not the difference between the model (unperturbed) energy of the excited state and the actual (perturbed) energy of the chosen configuration, as is done in the Brillouin-Wigner perturbation theory (see Sec. XIII, especially reference 50). The operator  $Q$  is defined as in Sec. III, below Eq. (3.1).

A slight modification, introduced in E,<sup>20</sup> is desirable. The actual nuclear wave function  $\Psi$  must of course satisfy the Schrödinger equation

$$E\Psi = H\Psi = \sum_i T_i \Psi + \sum_{ij} v_{ij} \Psi. \quad (4.5)$$

Now instead of requiring that (4.1) be true with  $\Phi$  the model wave function defined in Sec. II (which would require further modification of  $F$ ), we shall postulate that (4.2), (4.3) is the correct form of the model operator, but shall define a modified model wave function  $\Phi'$  by setting

$$\Psi = F\Phi'. \quad (4.6)$$

Following BL<sup>10</sup> and Eden,<sup>20</sup> we can then derive the Schrödinger equation for  $\Phi'$  as follows. Comparing (4.2)

and (4.3), we have

$$F = F_{ij} + \frac{Q}{e} I_{ij} F_{ij} \quad (4.7)$$

(no summation over  $ij$ ). Therefore

$$v_{ij} F = \left[ v_{ij} + v_{ij} \frac{Q}{e} (G_{ij} - \tilde{G}_{ij}) \right] F_{ij}, \quad (4.8)$$

where (4.4) has been used. The last term, with  $\tilde{G}_{ij}$ , will turn out to be an unimportant correction. The other terms may be combined by using the integral equation (3.7) for  $G$ , which has the form<sup>24</sup>

$$G_{ij} = v_{ij} + v_{ij} \frac{Q}{e} G_{ij}. \quad (4.9)$$

Therefore

$$v_{ij} F = G_{ij} F_{ij} - v_{ij} \frac{Q}{e} \tilde{G}_{ij} F_{ij} \quad (4.10)$$

$$= \tilde{G}_{ij} \left( F - \frac{Q}{e} I_{ij} F_{ij} \right) + I_{ij} F_{ij} - v_{ij} \frac{Q}{e} \tilde{G}_{ij} F_{ij}, \quad (4.11)$$

where we have again used (4.4) and (4.7). We now sum over  $ij$  and transform the third term of (4.11), using (4.2):

$$\begin{aligned} \sum I_{ij} F_{ij} &= \sum (1-Q) I_{ij} F_{ij} + \sum Q I_{ij} F_{ij} \\ &= \sum (1-Q) I_{ij} F_{ij} + e(F-1). \end{aligned} \quad (4.12)$$

Collecting all terms in (4.5) and (4.6), we have then

$$EF\Phi' = (\sum_i T_i + \sum_{ij} \tilde{G}_{ij} + e) F\Phi' - e\Phi' + w\Phi', \quad (4.13)$$

where  $w$  is an operator consisting of three parts,

$$w_1 = \sum_{ij} (1-Q) I_{ij} F_{ij}, \quad (4.14)$$

$$w_2 = - \sum_{ij} \tilde{G}_{ij} \frac{Q}{e} I_{ij} F_{ij}, \quad (4.15)$$

$$w_3 = - \sum_{ij} v_{ij} \frac{Q}{e} \tilde{G}_{ij} F_{ij}. \quad (4.16)$$

We shall now show that the terms involving  $F\Phi' = \Psi$  in (4.13) can be greatly simplified by proper choice of  $e$ . For this purpose, we consider  $\Psi = F\Phi'$  expanded in terms of the original model wave functions of Sec. II (Slater determinants). In order for this expansion to be useful, all the model wave functions (for all configurations  $B$ ) must satisfy the "model wave equation"

$$(E - H_B)\Phi_B = 0, \quad (4.17)$$

<sup>24</sup> It should be noted that the denominator here is  $e$  just as in (4.2) and (4.3). Thus excitations of nucleons other than  $i$  and  $j$  have to be included in  $e$ . This is in the spirit of Sec. III and different from E, Eq. (2.7). It avoids the last correction term in E, Eq. (2.15), which could give rise to a spurious dependence on higher powers of  $A$ .

where  $H_M$  is the "model Hamiltonian"

$$H_M = \sum T_i + \sum G_{ij}. \quad (4.18)$$

It will be shown in Sec. VII how  $\tilde{G}_{ij}$  must be defined in order that (4.17) be true. In particular, the nondiagonal elements of  $\tilde{G}_{ij}$  must be defined by (7.4) and (7.7), regardless of the excitation of nucleons other than  $i$  and  $j$ . This definition insures also that the  $\Phi_B$  form an orthogonal system. It should be noted that  $H_M$  has only diagonal elements with respect to the model wave functions  $\Phi_B$  but that  $\sum T_i$  and  $\sum \tilde{G}_{ij}$  alone would also have nondiagonal elements. Further, according to (7.3), the diagonal elements of  $\tilde{G}_{ij}$  are equal to those of  $G_{ij}$  and are to be calculated by solving (4.9), taking the excitations of all nucleons into account in the denominators  $e$ .

We now define the operator  $e$  also as diagonal in the model wave functions, thus

$$e = E_C - E_B, \quad (4.19)$$

where  $E_C$  is the model energy of the chosen configuration. Then (4.13) reduces to

$$(E - E_C)F\Phi' + e\Phi' = w\Phi'. \quad (4.20)$$

We can first determine  $E$ . Assuming that the chosen configuration is not degenerate, i.e., that the nucleus contains only closed shells (the more general case will be considered below), we project Eq. (4.20) on the model wave function of the chosen configuration,  $\Phi_C$ . From (4.19), we see that  $e=0$  in this case.

Further, from (4.2),

$$(\Phi_C, F\Phi') = (\Phi_C, \Phi'), \quad (4.21)$$

because  $Q=0$  in the configuration  $C$ . Therefore (4.20) yields<sup>25</sup>

$$E - E_C = (\Phi_C, w\Phi') / (\Phi_C, \Phi') = w_C. \quad (4.22)$$

This, together with (4.17) and (4.18), is the basis of Eq. (3.3). Equation (4.19) justifies our treatment of energy denominators in Sec. III. Further, (4.20), may be rewritten

$$e\Phi' = (w - w_C F)\Phi'. \quad (4.23)$$

The operator  $w - w_C F$  is small. Its diagonal matrix elements are zero by (4.22), and we therefore consider its nondiagonal elements

$$(\Phi_B, (w - w_C F)\Phi_C) \quad (4.24)$$

for states  $E_B \neq E_C$ . Then the contribution of  $w_1$  is zero

<sup>25</sup> The matrix elements here, and in the foregoing, must be taken with respect to the model wave functions  $\Phi_B$  because only in these is the operator  $e$  diagonal [see the derivation of (4.20)]. They must not be taken with respect to the complete nuclear wave function, and in particular (4.22) must not be replaced by

$(\Psi_C, w\Phi')$ , (a)

as BL do in their Eq. (25). The use of (4.22) is at the same time a great simplification of the calculation, and it greatly reduces the numerical value of the correction terms  $w_2$  and  $w_3$ , as will be shown in Sec. XIV.

because of the factor  $1-Q$ , that of  $w_2$  and  $w_3$  is extremely small according to Sec. XIV, and therefore (4.24) is proportional to  $w_C$ . This energy correction, however, is also small as will be shown in Sec. XII. Therefore, very nearly,

$$\Phi' \approx \Phi_C, \quad (4.25)$$

and (4.22) may be simplified to

$$w_C \approx (\Phi_C, w\Phi_C). \quad (4.26)$$

Now consider this expression, in particular the part due to  $w_1$  which will be shown in Sec. XII and XIV to be the most important contribution. The operator  $1-Q$  equals 1 in our case because the nucleus is ultimately in state  $C$ . Hence

$$(\Phi_C, w_1 \Phi_C) = (I_{ij}, \Phi_C, F_{ij}, \Phi_C). \quad (4.27)$$

Now when (4.27) is evaluated in a straightforward manner, certain terms appear which are proportional to  $A^2$  and higher powers of the number of nucleons  $A$  in the nucleus. These terms were discovered by Brueckner in his "linked cluster" paper,<sup>15</sup> BC, and shown by him to be spurious, i.e. to be compensated by other terms, *tiz.* the energy perturbations in the energy denominators. Brueckner's prescription is to take into account only linked clusters in the expression (4.26) for  $w_C$ .

For the purpose of defining linked clusters, we will regard  $F$  as the sum of the infinite series of terms which would be obtained by iteration of  $F_{ij}$  in (4.2) using (4.3). Each term consists of a sum of products of two-suffix symbols. We will consider one such product acting on a single term in the Slater determinant  $\Phi$ ; it will involve a series of suffixes  $ij, lm, pq, \dots$  and there will be no summation. We will say that the pair  $ij$  is "directly linked" to  $pq$  if either one of the numbers  $i, j$  is equal to either one of  $p, q$ . We will say that  $ij$  is "linked" to  $lm$  if in the term we are considering it is possible to go from  $ij$  to  $lm$  via a chain of directly linked pairs. The term will be called a "linked cluster" term if all pairs of suffixes in it are linked. Thus a third order term having suffixes  $ij, jk, kl$  is a linked cluster.

Brueckner, in BC, has shown that there should not be any contributions from "unlinked clusters" to the energy  $E$  of the nucleus. Unlinked clusters are the analog of "disconnected graphs" in field theory, which are known not to give any contribution in that theory. In our case also, they would be entirely unphysical, giving rise to the appearance of terms proportional to  $A^2$  and higher powers of  $A$  in the expression for the energy of the nucleus. Indeed, Brueckner shows by direct evaluation that at least up to fourth order of standard perturbation theory, the contributions from unlinked clusters actually cancel. This is a great advance over the Brillouin-Wigner formulation of perturbation theory in which these troublesome terms always occur.

Goldstone<sup>26</sup> has shown quite generally that unlinked clusters must be omitted, by direct application of field theoretic methods to the problem of the complex nucleus. His method is exact, and shows that  $w_c$  is given by (4.27) with the proviso that only linked clusters must be taken into account. The corrections  $w_2$  and  $w_3$  of (4.15), (4.16) do not appear but there are some minor modifications of the prescription for calculating the matrices  $G$  and  $\tilde{G}$ .

We shall now discuss the matrix elements

$$\langle \Phi_B, w_1 \Phi_C \rangle \quad (4.28)$$

in more detail. Because of the factor  $1 - Q$ , these elements are different from zero only if the state  $B$  has the same energy as the chosen configuration. We must therefore distinguish the two cases in which (a) the chosen configuration is degenerate with other states, and (b) it is nondegenerate. In case (b),  $w_1$  has only a diagonal element. Thus  $w_1$  will only contribute to the energy of the nucleus but will leave  $\Phi' = \Phi$ . It will be shown in Sec. XII that the diagonal element of  $w_1$  can arise only from the successive interaction of three or more nucleons (three-particle clusters). As a consequence, this term is rather small *per nucleon*, but it is proportional to the number of nucleons. It will change rather little from one configuration to another because it depends only on the behavior of the wave function when three nucleons come very close together, and not on its over-all behavior. Thus the diagonal term of  $w_1$  for any configuration may be replaced by a constant, *viz.*, its expectation value for the chosen configuration,  $w_{1c}$ . This result has been used in (3.5).

In case (a), the diagonal term will also arise and have substantially the same value as in case (b). But in addition, there are matrix elements of  $w_1$  linking the various degenerate configurations. For instance, all the degenerate configurations may have 3 nucleons in the  $1g$  shell, and differ by the magnetic quantum numbers assigned to these 3 nucleons. Then the operator  $I_{ij}$  may change the magnetic quantum numbers so as to cause a transition from one of the degenerate configurations to another. Thus  $w_1$  will in this case have nonvanishing matrix elements even if  $F_{ij}$  in (4.14) is replaced by unity, while in case (b) the matrix elements vanish if this replacement is made, because the diagonal elements of  $I_{ij}$  are zero by definition (see Sec. XII). The non-diagonal matrix elements of  $w_1$  between degenerate configurations are therefore apt to be considerably larger than the contribution of one pair  $ij$  to the diagonal element  $w_1$ . On the other hand, only the nucleons in incomplete shells will contribute to the nondiagonal elements, and therefore the nondiagonal elements of  $w_1$  will not be proportional to  $A$  but to a lower power of  $A$ . The nondiagonal elements can be treated by the usual methods of perturbation theory for degenerate states, as will be described in Sec. XVI.

<sup>26</sup> J. Goldstone, Proc. Roy. Soc. (London), (to be published).

The two perturbation terms  $w_2$  and  $w_3$  have already been treated by BL. They show that the diagonal matrix elements of  $w_2$  and  $w_3$  give a contribution to the energy which is independent of  $A$ , and is therefore of order  $1/A$  relative to the main binding energy of the nucleus. In Sec. XIV, we shall confirm this result and shall show that the numerical value of this contribution is much smaller than BL estimated, *viz.*, only a few hundred kev for the whole nucleus, rather than 10 Mev: hence the method remains good down to small nuclei.

The nondiagonal elements of  $w_2$  and  $w_3$  give contributions of order  $1/A$  to the energy and to the wave function, as will be shown in Sec. XIV. They are therefore entirely negligible.

#### V. DISCUSSION AND COMPARISON WITH THE HARTREE-FOCK METHOD

The actual wave function defined by (4.1) to (4.3) may be expanded in a series of terms involving no, one, two, . . . interactions. The first approximation to  $F$  is obtained if  $F_{ij}$  in (4.2) is replaced by unity. Then putting the nondiagonal elements of  $I_{ij}$  equal to those of  $G_{ij}$  (see Sec. VII), we get for the wave function of a nucleus containing  $A$  nucleons:

$$\Psi_C = \Phi(n_1^0, n_2^0, \dots, n_A^0) - \sum_{i < j} \sum'_{n_i} \sum'_{n_j} \frac{1}{\delta(n_i, n_j; n_i^0, n_j^0)} (n_i n_j | G_{ij} | n_i^0 n_j^0) \times \Phi(n_1^0, n_2^0, \dots, n_i, \dots, n_j, \dots, n_A^0). \quad (5.1)$$

Here the model wave functions have been explicitly designated by the configuration to which they belong, and the primes mean that the sums go only over unoccupied states  $n_i$ ,  $n_j$ . Terms including more than two excited nucleons have been omitted in (5.1). If  $G_{ij}$  were further approximated by  $v_{ij}$ , then this approximation would correspond to the first-order (not zero order) wave function of standard perturbation theory. Thus the wave function  $\Psi$  includes, besides the model wave function  $\Phi$ , also all states which can be generated from  $\Phi$  by letting an arbitrary pair of nucleons  $i$  and  $j$  scatter each other. In higher approximations, i.e., when  $F_{ij}$  from (4.3) is inserted into (4.2), multiple scattering is also taken into account (see below). Furthermore, the use of  $G_{ij}$  in (5.1) constitutes an improvement over the use of  $v_{ij}$  in first-order perturbation theory.

The Hartree-Fock method is obtained from the Brueckner method by the following approximations:

(1) The wave function is assumed to be  $\Phi$ , rather than  $\Psi$ .

(2) The second term in (3.1) is left out, i.e., the  $G$  matrix is replaced by the  $v$  matrix,  $(n'_i n'_j | v_{ij} | n_i n_j)_N$ . The Hartree approximation itself is obtained by the further approximation of replacing  $(n'_i n'_j | v_{ij} | n_i n_j)_N$  by  $(n'_i n'_j | v_{ij} | n_i n_j)_P$ , i.e., neglecting the exchange term in (2.6). Clearly, for nucleons which have exchange

forces between them, this would be a very poor approximation.

To see that the Brueckner method is a vast improvement over the Hartree-Fock approximation, we consider merely the first step in solving Eq. (3.1) by iteration, i.e., we replace  $G_{ij}$  in the sum in (3.1) by  $v_{ij}$ . (The Hartree-Fock approximation would be obtained by neglecting the sum altogether.)

Let  $n_i = n_i^0$  and  $n_j = n_j^0 = n_i^0$ , where  $n_i^0, n_j^0$  denote as usual the states of nucleons  $i$  and  $j$  in the chosen configuration. Sum over all pairs of nucleons  $i, j$ . Then, according to (3.10), the left-hand side of (3.1) will yield the total potential energy of the nucleus,  $E_{\text{pot}}^{(2)}$ , the superscript 2 indicating that this is the second approximation. We find

$$E_{\text{pot}}^{(2)} = E_{\text{pot}}^{(1)} + \sum_B Q \frac{|(B|W|C)|^2}{E_C - E_B}, \quad (5.2)$$

where  $E_{\text{pot}}^{(1)}$  is the first (Hartree-Fock) approximation to the potential energy,  $C$  is the "chosen" configuration of the nucleus,  $B$  any excited configuration,

$$W = \sum_{ij} v_{ij} \quad (5.3)$$

is the sum of the interaction operators over all nucleon pairs. Clearly (5.2) is exactly the second-order perturbation theory result for the potential energy, and the second term is the full "configuration interaction," summed over *all* excited configurations which can be reached by the excitation of two nucleons from the chosen configuration. Thus (5.2) is a far better approximation than has ever been attempted in calculating either atomic or nuclear energy levels, and it is only the first step of the Brueckner method in improving the Hartree-Fock approximation.

A great advantage of the use of the scattering matrix  $G$ , instead of a perturbation expansion, will be that unpleasant divergences common in perturbation theory may be avoided. The case of the greatest practical importance in nuclear physics is that of a repulsive core, i.e., an infinite repulsive potential for  $r < a$ . Then the matrix elements of the interaction  $v$  are infinite, but the elements of the scattering matrix  $G$  are finite.<sup>23</sup> There are probably also advantages in the treatment of Coulomb interactions.

The wave function (5.1) also contains configuration interaction. This is true in spite of the fact that in (5.1) the crude approximation has been made of replacing  $F_{ij}$  by unity, which means the neglect of multiple scattering. But even in this crude approximation, the wave function contains strong two-particle correlations between the nucleons, and thus is much superior to the Hartree-Fock wave function. Moreover, it contains the high-momentum components which are required by high-energy experiments, as discussed in Sec. I and by Brueckner, Eden, and Francis.<sup>7</sup>

Thus the Brueckner method gives an improvement, both of the wave function and of the energy, over the

Hartree-Fock method. In the Hartree-Fock method, the motion of *one* particle is considered in the average potential produced by all the others. In the Brueckner method, the interaction of *two* particles is calculated accurately, and only the influence of the third and further particles is replaced by an average potential. Thus the Brueckner method is a logical extension of the Hartree method; the price for its increased power and accuracy is of course the increased complication in the determination of the self-consistent field (see Sec. III).

Perhaps the most important advance is that in the Brueckner method the error can in principle be calculated, by evaluating the matrix elements of the perturbations (4.14) to (4.16) between model wave functions. In the Hartree method, the error has always been assumed to be small, and has turned out to be small in practical applications to atoms, but no method was available heretofore to estimate the error quantitatively.

The Brueckner theory is simplified, and made more similar to the Hartree-Fock theory, if it is possible to make the approximation (3.8), i.e., to assign to each nucleon an energy  $E(n_i)$  as given by (3.11). One may then identify the second term in (3.11) with the potential energy of nucleon  $i$  and set

$$V(n_i) = \sum_j (n_i n_j^0 | G_{ij} | n_i n_j^0). \quad (5.4)$$

For the occupied states  $n_i = n_i^0$ , as was mentioned in (3.9), the matrix elements of  $G_{ij}$  occurring in (5.4) are always well defined and therefore the definitions (5.4), (3.11) are sensible. BL assumed (5.4) to be correct for all states.

The total energy of the nucleus is given by (3.3). Neglecting  $w_{1c}$ , we obtain the model energy, but this is still not equal to the sum of the eigenvalues  $E(n_i)$  of all the nucleons, because in (3.3) each pair  $ij$  must be counted only once while summation of (5.4) over all  $i$  would count each pair  $i,j$  twice. We have for the total model energy

$$E = \sum_i (n_i | T_i | n_i) + \frac{1}{2} \sum_i (n_i | V | n_i) \quad (5.5)$$

$$= \sum_i E(n_i) - \frac{1}{2} \sum_i (n_i | V | n_i). \quad (5.6)$$

The factor  $\frac{1}{2}$  in (5.5), and the subtracted term in (5.6), are of course very familiar from the ordinary Hartree model, but nevertheless seem always to create some difficulty. Further discussion will be found in Sec. IX.

As has been stated, (5.4) and (3.11), and therefore (5.5) and (5.6), are strictly applicable only to the chosen configuration; for excited nucleons, the  $G_{ij}$  in (5.4) depends actually on several additional quantum numbers.

## VI. ACTUAL AND MODEL WAVE FUNCTIONS

It is interesting to ask how closely the actual wave function  $\Psi_c$  is approximated by the model wave function  $\Phi_c$ . For this purpose, we consider the actual

wave function expanded in model wave functions,

$$\Psi_C = \sum c_B \Phi_B, \quad (6.1)$$

$$c_B = (\Phi_B, \Psi_C).$$

To calculate the expansion coefficients, we use the expressions (4.1)–(4.3) for  $\Psi_C$  whose first three terms are

$$\Psi_C = \Phi_C + \sum_e \frac{\Omega}{I_{ij}} \Phi_{Cj} + \sum_e \sum_m \frac{\Omega}{I_{ij}} \frac{\Omega}{I_{im}} \Phi_{Cm} + \dots \quad (6.3)$$

The second term expresses one, the third term two scatterings.

To obtain  $c_B$ , it is convenient to consider a nucleus of given volume  $\Omega$  and number of particles  $A$ . Both are assumed large and proportional to each other. We then wish to calculate the dependence of the various terms on  $\Omega$ . Since  $\Omega$  is assumed large, momentum will be almost conserved in the matrix elements of  $I_{ij}$  (see Sec. XV). These will of course have the same dependence on  $\Omega$  as  $v_{ij}$ ; the latter is given by

$$\begin{aligned} & \langle \mathbf{k}_i' | v_{ij} | \mathbf{k}_i \mathbf{k}_j \rangle \\ &= \int \psi^*(\mathbf{k}_i', \mathbf{r}_i) \psi^*(\mathbf{k}_j', \mathbf{r}_j) v_{ij}(\mathbf{r}_{ij}) \\ & \quad \times \psi(\mathbf{k}_i, \mathbf{r}_i) \psi(\mathbf{k}_j, \mathbf{r}_j) d\mathbf{r}_i d\mathbf{r}_j; \\ &= \Omega^{-2} \int e^{-i\mathbf{k}_i' \cdot \mathbf{r}_i - i\mathbf{k}_j' \cdot \mathbf{r}_j} e^{i\mathbf{k}_i \cdot \mathbf{r}_i + i\mathbf{k}_j \cdot \mathbf{r}_j} \\ & \quad \times v_{ij}(\mathbf{r}_{ij}) d\mathbf{r}_i d\mathbf{r}_j. \end{aligned} \quad (6.4)$$

The factor  $\Omega^{-2}$  comes from the normalization of the wave functions, each of the four wave functions having a normalization factor  $\Omega^{-1}$ . Now in the last form of the integral, the exponential is  $\exp[i(\mathbf{k}_i - \mathbf{k}_i') \cdot (\mathbf{r}_i - \mathbf{r}_j)]$ , considering that  $\mathbf{k}_i - \mathbf{k}_i' = \mathbf{k}_j - \mathbf{k}_j'$  by momentum conservation. Then, holding the relative coordinate  $\mathbf{r}_i - \mathbf{r}_j$  fixed, we may integrate over  $d\mathbf{r}_i$  and obtain a factor  $\Omega$  while the integral over  $\mathbf{r}_i - \mathbf{r}_j$  gives a factor independent of  $\Omega$ . Thus

$$I_{ij} \sim v_{ij} \sim \Omega^{-1}. \quad (6.5)$$

Essentially the same result would be obtained for a finite nucleus, i.e., if the wave functions  $\psi$  are not exactly plane waves in the volume  $\Omega$  but tail off at the surface.

If we consider two definite nucleons  $\mathbf{k}_i, \mathbf{k}_j$ , then the amplitude of the model state in which  $\mathbf{k}_i$  has been changed to  $\mathbf{k}'_i$  by means of the term  $I_{ij}$  in (6.1) is proportional to  $\Omega^{-1}$ , and the "probability" of finding the nucleus in this state is therefore proportional to  $\Omega^{-2}$ . Now for given  $\mathbf{k}_i$  and  $\mathbf{k}_j$ , the final state  $\mathbf{k}'_i$  can be chosen freely, and the number of possible quantum states  $\mathbf{k}'_i$  per unit volume in momentum space is proportional to  $\Omega$ . The other final state  $\mathbf{k}'_j$  is determined by momentum conservation. Thus for given  $i$  and  $j$ , the number of possible "final" states is proportional to  $\Omega$  and the total probability of exciting any of these

is therefore proportional to  $\Omega^{-1}$ . Since the number of pairs of nucleons  $ij$  is proportional to  $\Omega^2$ , the total probability of finding the nucleus in an excited model state is proportional to  $\Omega$ , the probability of the chosen state being set equal to 1. Of course this takes into account only the action of the second term in (6.1). Since  $\Omega$  is proportional to  $A$ , we may set the probability of an excited model state equal to  $\alpha A$ , where  $\alpha$  is a numerical coefficient depending on the actual nuclear forces.

We can easily generalize this result, especially if we assume that there are no linked clusters containing more than two particles each. Then (6.1) is equivalent to a product over all possible pairs of particles,

$$F = \prod_{ij} \left( 1 + \frac{\Omega}{e} I_{ij} \right). \quad (6.6)$$

Each term gives a probability  $2\alpha/A$  for finding just the pair  $ij$  excited, with  $\alpha$  defined in the last paragraph. Since there are  $\frac{1}{2}A^2$  pairs, the total probability of finding any pair excited is  $e^{-\alpha A}$  if we still set the probability of the chosen model state equal to 1. However, it is more convenient to change the normalization and to set the total probability of any model state equal to one. Then the probability of "finding" the nucleus "actually" in the state described by the model wave function is

$$|\langle \Phi_C, \Psi_C \rangle|^2 \sim e^{-\alpha A}. \quad (6.7)$$

This is exponentially small for a large nucleus. Therefore it would be entirely wrong to say that a large nucleus is "actually" in its model state; the probability for this is "infinitesimal," and is smaller the larger the nucleus. The result (6.7) is not changed if clusters of three or more particles are taken into account, except of course for the value of  $\alpha$ .

The difficulty of many<sup>27</sup> "old-fashioned" treatments of nuclear structure was that they attempted to obtain the actual nuclear wave function  $\Psi_C$  which is complicated when expressed in model functions  $\Phi_C$ . The great achievement of the Brueckner theory is that it permits the calculation of energy levels and other nuclear properties in terms of the model function of the chosen configuration,  $\Phi_C$ . For the energy this has already been demonstrated. We shall now discuss other properties.

The most important observable properties of a nucleus (other than the energy) depend on one-nucleon operators, such as the magnetic moment which is the sum of the magnetic moment operators of the individual nucleons, the dipole moment for an optical transition between two nuclear levels, or the momentum distribution of a nucleon which influences some of the experi-

<sup>27</sup> Swiatecki (to be published) has shown, however, that the energy of a nucleus may be obtained by ordinary perturbation theory provided the interaction between nucleons is well-behaved, and that then each term in the perturbation expansion is proportional to  $A$ .

ments mentioned in Sec. I. We shall therefore consider the evaluation of one-nucleon operators, in particular of the diagonal matrix elements for the chosen configuration of an operator  $M = \sum M_i$ , where  $M_i$  is a one-nucleon operator such as the magnetic moment; we have

$$\langle M \rangle = \sum_i (\Psi_C, M_i \Psi_C) / (\Psi_C, \Psi_C). \quad (6.8)$$

We consider  $\Psi_C$  expanded in terms of model wave functions. Then, because of the orthogonality of the model wave functions,

$$\begin{aligned} (\Psi_C, M_i \Psi_C) &= \sum_B \sum_{n_i} \sum_{n'_i} (\Psi_C, \Phi_{Bn_i}) \\ &\quad \times (\Phi_{Bn'_i}, \Psi_C) (\psi_{n'_i}, M_i \psi_{n_i}), \end{aligned} \quad (6.9)$$

where  $B$  is a configuration of the  $A-1$  nucleons other than  $i$ , and  $Bn_i$  denotes the configuration of our nucleus in which the  $A-1$  nucleons are in configuration  $B$  and nucleon  $i$  in state  $n_i$ . The last factor in (6.9) depends only on the states of nucleon  $i$ ; it is immaterial whether the other nucleons are excited or not. We are therefore only interested in

$$\sum_B (\Psi_C, \Phi_{Bn_i}) (\Phi_{Bn'_i}, \Psi_C), \quad (6.10)$$

which represents essentially the probability that one particular nucleon  $i$  is excited. This probability is of the order of magnitude one, regardless of the size of the nucleus. This follows from (6.7); the desired probability (6.10) will be the ratio of the excitation probability for all nucleons,  $e^A$ , to that for  $A-1$  nucleons,  $e^{A(A-1)}$ , giving  $e^a$  which is independent of  $A$ .

This result makes it possible to calculate the expectation value (6.8) with a finite amount of labor. To carry out such a calculation, it will probably be convenient to use the same techniques as have been applied in field theory, especially the method of Feynman diagrams.<sup>26</sup> The chosen configuration corresponds to the vacuum state in field theory; a transition of one particle is considered as the creation of a pair, consisting of a hole in the state  $n_i^0$  of the chosen configuration and of a particle in the state  $n'_i$  outside the Fermi sphere. The interaction  $\tau_{ij}$  or  $G_{ij}$  connects two particle lines. The operator  $M$  is then an additional operator which may be inserted in one of the particle lines; it is similar to the action of an external potential in field theory.

The analogy with field theory is close. The physical vacuum state has only an infinitesimal projection on the bare vacuum state, just as the actual wave function  $\Psi_C$  of the nucleus has only a very small projection on the model state  $\Phi_C$ , Eq. (6.7). Nevertheless, the properties of single electrons (such as their magnetic moment), or the interaction of two particles, can be derived in field theory by considering just these particles themselves and a limited number of photons, electron pairs, etc. with which they interact directly. One may disregard all disconnected diagrams and in the nuclear case all unlinked clusters.

## VII. DEFINITION OF THE MATRICES $\bar{G}$ AND $I$

While the reaction matrix  $G$  is defined by Sec. III, particularly by Eqs. (3.1) and (3.7), there is still some arbitrariness in the definition of the matrix  $\bar{G}$  and hence of  $I$ , Eq. (4.4). There is further arbitrariness in the one-nucleon potential  $V$ . This can be used to make the operator in (4.13),

$$\sum_i T_i + \sum_i \bar{G}_{ii} \quad (7.1)$$

diagonal in the model wave functions. Then  $e$  in (4.3) becomes a number, i.e.,  $e$  is also diagonal in the model wave functions. Furthermore, it is desirable to choose  $I_{ij}$  such that it has no diagonal matrix elements, and no matrix elements leading from the chosen configuration to configurations in which only one nucleon is excited, because this choice will greatly reduce the number of terms which needs to be considered in the perturbations  $w_1$  to  $w_3$ , Eqs. (4.14) to (4.16).

We thus set

$$(n_i n_j | I_{ij} | n_i n_j) = 0, \quad (7.2)$$

$$(n_i n_j | \bar{G}_{ij} | n_i n_j) = (n_i n_j | G_{ij} | n_i n_j), \quad (7.3)$$

where, if  $n_i$  and/or  $n_j$  are normally unoccupied, the right-hand side of (7.3) should still depend on the states left empty in the chosen configuration (see Sec. III). The choice (7.3) actually does not affect the above condition that (7.1) should be diagonal; the diagonal elements of (7.1) can be chosen arbitrarily without violating this condition.

Since the one-nucleon wave functions are orthogonal, the only nonvanishing elements of the operator  $T_i$  are (a) the diagonal elements and (b) elements in which the state of nucleon  $i$  changes and all other nucleons remain in the same state. Therefore  $\bar{G}$  must not have any elements in which both nucleons  $i$  and  $j$  change their state,

$$(n'_i n'_j | \bar{G}_{ij} | n_i n_j) = 0 \quad \text{if } n'_i, n'_j \neq n_i, n_j, \quad (7.4)$$

$$\begin{aligned} (n'_i n'_j | I_{ij} | n_i n_j) &= (n'_i n'_j | G_{ij} | n_i n_j) \\ &\quad \text{if } n'_i, n'_j \neq n_i, n_j. \end{aligned} \quad (7.5)$$

$$\begin{aligned} &\text{If one nucleon } (i) \text{ changes its state, we must have} \\ &(n'_i | T_i | n_i) + \sum_j (n'_i n_j | \bar{G}_{ij} | n_i n_j) = 0, \quad \text{if } n'_i \neq n_i. \end{aligned} \quad (7.6)$$

Thus the sum in (7.6) must be chosen to be independent of the states occupied by the other nucleons, and it is most convenient to set

$$(n'_i n_j | \bar{G}_{ij} | n_i n_j) = (n'_i n_j^0 | G_{ij} | n_i n_j^0) \quad \text{if } n'_i \neq n_i, \quad (7.7)$$

whether or not  $n_i = n_i^0$ , and whether or not all the other nucleons  $k$  are in the chosen configuration. However, as we have shown in Sec. III, the right hand side of (7.7) is still not defined if both  $n_i$  and  $n'_i$  differ from the chosen state  $n_i^0$ ; but if either of them is equal to  $n_i^0$ , there is no ambiguity; in the other case, we may choose an arbitrary state  $n^0$  to be empty, but this must be taken to be the same state for all matrix elements of type

(7.7), i.e., independent of  $i$ . Once  $\tilde{G}$  is chosen,  $I$  is determined by (4.4); in particular, (7.7) gives

$$\langle n_i n_j^0 | I_{ij} | n_i^0 n_j^0 \rangle = 0 \quad \text{if } n_i \neq n_j^0. \quad (7.8)$$

Thus the elements of  $I$  which start from the chosen configuration and go to configurations with only one nucleon excited are indeed zero as desired.

Since the model wave functions are orthogonal and the one-nucleon wave functions satisfy the Schrödinger equation (2.3), we have

$$\langle n' | T | n \rangle + \langle n' | V | n \rangle = 0 \quad \text{if } n' \neq n. \quad (7.9)$$

In order to satisfy (7.6), (7.9), and (7.7), we must choose the one-nucleon potential such that

$$\langle n' | V | n \rangle = \sum_j \langle n' n_j | \tilde{G}_{ij} | nn_j \rangle \quad (7.10)$$

$$= \sum_j \langle n' n_j^0 | G_{ij} | nn_j^0 \rangle. \quad (7.11)$$

This result was already used in (3.12). The matrix elements of  $V$  must of course be independent of the choice of the particular nucleon  $i$  in (7.7); therefore the sum in (7.10) must not exclude any nucleon  $j$ . If either  $n$  or  $n'$  is equal to  $n_i^0$ , the term  $j=i$  in (7.11) vanishes automatically because of the Pauli principle, so that there is no difficulty in this case. Thus the matrix elements of  $V$  between an occupied and an empty state are uniquely and reasonably defined by (7.11) and depend only on the initial and final state of a single nucleon. Those between two empty states cannot be uniquely defined as was shown in (3.13); since  $G$  is not a proper two-nucleon operator,  $V$  cannot be a proper one-nucleon operator. This ambiguity can only be resolved by arbitrary choice of these elements of  $V$ , but this choice has only little influence on the one-nucleon wave functions (end of Sec. III).

It will be shown in Sec. XV that the nondiagonal matrix elements of  $V$  and  $T$ , and the elements of  $G_{ij}$  in which only one nucleon changes its state, are small, of order  $\Omega^{-1}$  or less compared with the other matrix elements.

### VIII. SPIN CONSIDERATIONS

In this section we wish to evaluate the matrix elements of the interaction,

$$\langle n_i^0 n_j^0 | v_{ij} | n_i n_j \rangle_N, \quad (8.1)$$

and in particular to evaluate the sums over spin and charge of the two nucleons. We are particularly interested in the case when  $n_i, n_j$  are the states of particles  $i$  and  $j$  in the chosen configuration, although nearly all our results will also apply to more general cases. If  $n_i = n_i^0$  and  $n_j = n_j^0$ , then (8.1) corresponds to the removal from the chosen configuration of the nucleons in states  $n_i^0$  and  $n_j^0$ , and their placing into the states  $n_i^0 n_j^0$ , so that the final configuration is defined by four quantum numbers,  $n_i^0 n_j^0 n_i^0 n_j^0$ , which describe the states empty in the chosen configuration and those occupied outside that configuration. The states  $n_i^0 n_j^0$

should therefore be considered as having definite spins and charges, these being determined by the spins and charges of the nucleons which are left in the same orbitals (spatial wave functions) after  $n_i^0$  and  $n_j^0$  have been removed.<sup>28</sup>

We shall denote the spatial wave function (orbital) of the nucleon state  $n_i$  by  $m_i$ , the spin state by  $\alpha_i$ , and the charge state by  $\gamma_i$ , and similarly for the states  $n_j^0$ ,  $n_j^0$ , and  $n_j^0$ . Whenever we need to specify *definite* values of spin or charge, we call the spin wave functions  $\alpha$  and  $\beta$ , and the charge wave functions  $\gamma$  and  $\delta$ . The interaction will be written for the present as

$$v_{ij} = v_1 + v_2 \sigma_i \cdot \sigma_j, \quad (8.2)$$

where  $v_1$  and  $v_2$  depend on the spatial coordinate  $r_{ij}$ , but may still contain a Majorana exchange operator  $P_M$ . As is well known, the symmetry of the nuclear wave function in  $i$  and  $j$  needs to be taken into account only once, and we choose to do this in the final state; thus we take the initial state to be

$$|n_i n_j\rangle = m_i \alpha_i \gamma_i (i) m_j \alpha_j \gamma_j (j), \quad (8.3)$$

and the final state

$$|n_i^0 n_j^0\rangle = m_i' \alpha'_i \gamma'_i (i) m_j' \alpha'_j \gamma'_j (j) - m_i' \alpha'_i \gamma'_j (i) m_j' \alpha'_j \gamma'_i (j). \quad (8.4)$$

With these definitions, no normalizing factor  $1/\sqrt{2}$  is required. Finally, in applying (8.2) to (8.3), it is useful to distinguish immediately the cases when the two particles have equal or opposite spin.

A. Initial spin equal,  $\alpha_i = \alpha_j = \alpha$  (this is not meant to imply that the spin is necessarily up). Then also in the final state we must have  $\alpha'_i = \alpha'_j = \alpha$ ; otherwise the matrix element will vanish. Then, without loss of generality, we may set  $\gamma'_i = \gamma_i$ ,  $\gamma'_j = \gamma_j$  (if  $\gamma_i = \gamma_j$ , this makes no difference; if  $\gamma_i \neq \gamma_j$ , this defines which state is called  $n'_i$ ). The application of (8.2) to (8.3) gives

$$\langle n_i^0 n_j^0 | v_{ij} | n_i n_j \rangle = (v_1 + v_2) m_i (i) m_j (j) \alpha \gamma_i (i) \alpha \gamma_j (j) \quad (8.5)$$

and the matrix element with (8.4) is

$$\begin{aligned} \langle n_i^0 n_j^0 | v_{ij} | n_i n_j \rangle &= (m_i' (i) m_j' (j), (v_1 + v_2) m_i (i) m_j (j)) \\ &\quad - (\gamma_i \gamma_j) (m_i' (i) m_j' (j), (v_1 + v_2) m_i (i) m_j (j)). \end{aligned} \quad (8.6)$$

The scalar product  $(\gamma_i \gamma_j)$  is 1 if  $\gamma_i = \gamma_j$  and 0 if  $\gamma_i \neq \gamma_j$ ; thus the second (exchange) term in (8.6) will be present only when the two interacting nucleons have initially the same charge as well as the same spin. The matrix elements remaining unevaluated in (8.6) are purely spatial matrix elements, for which we write in abbreviated notation:

$$\langle n_i^0 n_j^0 | v_{ij} | n_i n_j \rangle = (v_1 + v_2)_D - (\gamma_i \gamma_j) (v_1 + v_2)_X. \quad (8.7)$$

<sup>28</sup> I am indebted to J. Goldstone for pointing out that the wave function of the two "removed" nucleons,  $i, j$  should not be symmetrized by itself in spin, charge, and space, because this is in general incompatible with leaving the "residual nucleus" after removal of  $i$  and  $j$  in a definite configuration.

$D$  meaning "direct" and  $X$  "exchange." It should be noted that in the final state spin and charge of both particles  $i, j$  are the same as in the initial state.

B. Initial spins different,  $\alpha_i = \alpha, \alpha_j = \beta$ . Then without loss of generality we set  $\alpha'_i = \alpha, \alpha'_j = \beta$ , thus defining which of the two final states is  $n'_i$ . Application of (8.2) on (8.3) gives

$$\begin{aligned} v_{ij}|n_i n_j\rangle &= (v_1 - v_2)m_i(i)m_j(j)\alpha\gamma_i(i)\beta\gamma_j(j) \\ &\quad + 2v_2m_i(i)m_j(j)\beta\gamma_i(i)\alpha\gamma_j(j). \end{aligned} \quad (8.8)$$

We then have to distinguish two cases for the charges.

1. Initial charges equal,  $\gamma_i = \gamma_j = \gamma$ . Then also the final charges must be  $\gamma'_i = \gamma'_j = \gamma$ . Using (8.4), the matrix elements are found to be

$$(n'_i n'_j | v_{ij} | n_i n_j) = (v_1 - v_2)_D - 2v_{2X}. \quad (8.9)$$

2. Initial charges different,  $\gamma_i = \gamma$  and  $\gamma_j = \delta$ . This is the only case where two different final states are possible:

(a) Final charges = initial charges,  $\gamma'_i = \gamma, \gamma'_j = \delta$ . Then

$$(n'_i n'_j | v_{ij} | n_i n_j) = (v_1 - v_2)_D. \quad (8.10)$$

(b) Charges interchanged in final state,  $\gamma'_i = \delta, \gamma'_j = \gamma$ . Then

$$(n'_i n'_j | v_{ij} | n_i n_j) = -2v_{2X}. \quad (8.11)$$

It is convenient now to introduce the interaction in singlet and triplet state,  $v_s$  and  $v_t$ , instead of  $v_1$  and  $v_2$ . We have

$$v_t = v_1 + v_2, \quad (8.12)$$

$$v_s = v_1 - 3v_2, \quad (8.13)$$

and we get from (8.7) to (8.11) the following matrix elements:

1. Charges and spins equal for both nucleons, wave functions  $\alpha\gamma, \alpha\gamma$  (both initially and finally):

$$v_{ij} = v_{tD} - v_{sX}. \quad (8.14)$$

2. Spins equal, charges different, wave functions  $\alpha\gamma, \beta\delta$  (initially and finally):

$$v_{ij} = v_{tD}. \quad (8.15)$$

3. Spins different, charges equal, wave functions  $\alpha\gamma, \beta\gamma$  (initially and finally):

$$v_{ij} = \frac{1}{2}(v_{tD} + v_{sD}) + \frac{1}{2}(v_{sX} - v_{tX}). \quad (8.16)$$

4. Spins and charges different, initial wave functions  $\alpha\gamma, \beta\delta$ ; (a) final wave functions the same  $\alpha\gamma, \beta\delta$ :

$$v_{ij} = \frac{1}{2}(v_{tD} + v_{sD}). \quad (8.17)$$

(b) final charges interchanged, wave function  $\alpha\delta, \beta\gamma$ :

$$v_{ij} = \frac{1}{2}(v_{sX} - v_{tX}). \quad (8.18)$$

The most important matrix element is the diagonal one, summed over all spins and charges of nucleon  $j$ , keeping those of nucleon  $i$  fixed. This is obtained by

summing Eqs. (8.14) to (8.17) which yields

$$\sum_{\text{spin, charge}} v_{ij} = 3v_{tD} + v_{sD} + \frac{1}{2}v_{sX} - \frac{1}{2}v_{tX}. \quad (8.19)$$

The coefficients, 1 and 3, of  $v_s$  and  $v_t$ , are the statistical weights. The signs of the exchange terms reflect the symmetry of the spatial wave function. The factors  $\frac{1}{2}$  with the exchange terms arise from the fact that these terms exist only between two like nucleons.

If the two nucleons are to be followed from the chosen configuration through a set of intermediate states and back to the chosen configuration, their spins and charges are, in most cases, simply left unchanged in the process. Only in the single case when both spin and charge are initially different, two kinds of intermediate states must be considered: the two nucleons may retain spin as well as charge, or else they may retain their spins but exchange their charges. The latter elements will be absent if  $v_{sX} = v_{tX}$ , i.e., in particular if the triplet and singlet forces are assumed to be the same. This is not a bad approximation to the known interaction in the  $S$  state. The forces in the odd-parity states of two nucleons are not sufficiently well known to decide whether  $v_s = v_t$  is a good approximation.

If the equation for the scattering matrix, (3.1), is solved by iteration, as in Sec. X, then in the second approximation the effect of a pair of intermediate orbitals  $m'_i m'_j$  will be given by the sum of the squares of the matrix elements (8.14) to (8.18). Although the result is elementary we shall not give it, but shall first simplify our assumptions about the interaction.

We assume now that the spatial dependence of the interaction is that of a Serber force, i.e.,

$$v_{ij}(r_{ij}) = v(r_{ij}) \frac{1}{2}(1 + P_M), \quad (8.20)$$

where  $P_M$  is the Majorana exchange operator. As is well known, the Serber force is zero for all two-nucleon states of odd parity (odd orbital momentum), while for even parity it is simply  $v(r_{ij})$ . Later on (Sec. XI) we shall consider the assumption that there is interaction only in  $S$  states; this is a special case of the Serber force for which the following equations, especially (8.28), remain valid, although the analytic form (8.20) is not.

If (8.20) is assumed, then

$$\begin{aligned} v_D = v_X &= \frac{1}{2}(m'_i m'_j | v(r_{ij}) | m_i m_j) \\ &\quad + \frac{1}{2}(m'_i m'_j | v(r_{ij}) | m_i m_j), \end{aligned} \quad (8.21)$$

where the right-hand terms are ordinary spatial matrix elements,

$$\begin{aligned} (m' n' | v(r_{ij}) | mn) &= \int \psi_{m'}^*(\mathbf{r}_i) \psi_{n'}^*(\mathbf{r}_j) \\ &\quad \times v(r_{ij}) \psi_m(\mathbf{r}_i) \psi_n(\mathbf{r}_j) d\tau_i d\tau_j. \end{aligned} \quad (8.22)$$

Because of the equality  $v_D = v_X$ , the matrix elements (8.14) to (8.18) simplify considerably:

1. Spin and charge of the two nucleons equal:

$$v_{ij} = 0. \quad (8.23)$$

There is, in this case, no interaction because the Pauli principle requires the spatial wave function to be antisymmetric which makes it odd parity.

2. Spin equal, charge different:

$$v_{ij} = v_t. \quad (8.24)$$

3. Spin different, charge equal:

$$v_{ij} = v_s. \quad (8.25)$$

Pauli principle, and even parity of the spatial wave function (Serber force) together require an antisymmetric spin function, hence a singlet state.

4. Spin and charge different.

- (a) Final wave function same as initial:

$$v_{ij} = \frac{1}{2}(v_t + v_s). \quad (8.26)$$

- (b) Final wave function has charges interchanged:

$$v_{ij} = \frac{1}{2}(v_t - v_s). \quad (8.27)$$

The sum over all diagonal elements, (8.23) to (8.26), which was previously given by (8.19), now simplifies to

$$\sum v_{ij} = \frac{1}{2}(v_t + v_s). \quad (8.28)$$

This permits a simple interpretation: we consider the interaction of a given nucleon  $i$  with all the four nucleons in the orbital  $m_i$ . This is found to be effectively equal to the interaction with three nucleons, since that with the nucleon of the same spin and charge is exactly zero, Eq. (8.23). The effective interaction with each of the three nucleons is the average of the triplet and the singlet interaction. This is related to the fact that for even parity, there are equally many triplet as singlet states. This may be seen by considering the 16 possible spin-charge states of two nucleons: ten of these have symmetric spin-charge wave function and hence antisymmetric spatial wave functions, i.e., odd parity (9 of these have isotopic spin  $T=1$  and spin  $S=1$  while one has  $T=0, S=0$ ). Six states have antisymmetric spin-charge wave function, of which 3 are  $T=1, S=0$  and three are  $T=0, S=1$ .

We mentioned previously that the second-order contribution to the scattering matrix from an intermediate orbital  $m_i'$  is given by the sum of the squares of the matrix elements, in our case (8.23) to (8.28). This yields

$$\sum (v_{ij})^2 = \frac{1}{2}(v_t^2 + v_s^2). \quad (8.29)$$

Since the observed interaction is not very different in triplet and singlet even states, no great error will be made if  $\frac{1}{2}(v_t^2 + v_s^2)$  is replaced by the square of the average interaction,  $\frac{1}{2}(v_t + v_s)$ .

Throughout this paper, we shall therefore adopt the following simplified procedure. We replace the nuclear matrix elements of  $v$  by the average of singlet and triplet interaction for states of even parity. With these

elements of  $v$ , we then calculate the  $G$  matrix, using (3.1). From  $G$  we obtain the effective one-particle potential  $V$  by assuming that each nucleon interacts only with 3 out of 4 of the other nucleons (i.e., with 3 nucleons in each orbital  $m_i$ ).

Although we shall use the Serber interaction throughout this paper, it is still interesting to write down the average interaction (8.19) for the more general case when there is a Serber interaction  $v_s$  in even states and another interaction  $v_o$  in states of odd parity. Thus we write

$$v_{iD} = v_{ts} + v_{so}, \quad v_{iX} = v_{te} - v_{eo}, \quad (8.30)$$

and similarly for the singlet. Then (8.19) becomes

$$\sum v_{ij} = \frac{1}{2}v_{ts} + \frac{1}{2}v_{eo} + (9/2)v_{so} + \frac{1}{2}v_{eo}. \quad (8.31)$$

Thus each type of state contributes according to its statistical weight, the triplet odd states being  $T=S=1$  (weight 9) and the singlet odd ones  $T=S=0$  (weight 1, see above).

## IX. INFINITE NUCLEUS

The simplest case to which the theory can be applied is that of an infinite nucleus, in other words of nuclear matter. Clearly, the Coulomb interaction must be neglected in order to get finite results. In this case, the state of nuclear matter is fully characterized by its density (or more generally, by the neutron and proton density separately).

All positions are equivalent, and the proper wave functions are obviously plane waves. This obviates what is normally a most difficult part of determining the self-consistent field, *viz.*, the search for proper wave functions. The energy of a nucleon in the chosen configuration, which in Eq. (3.11) was shown to depend only on the state  $n_i^0$  of that nucleon, will now depend only on its momentum  $k$ , and we may write

$$E(k) = V(k) + k^2/2M. \quad (9.1)$$

In other words, the "self-consistent potential"  $V$  is now diagonal in a momentum representation,

$$\langle \mathbf{k}' | V | \mathbf{k} \rangle = V(k)(2\pi)^3 \delta(\mathbf{k} - \mathbf{k}'). \quad (9.2)$$

The self-consistent field problem then consists primarily in finding  $V(k)$ . It may be noted that we have here a situation opposite to that of the conventional Hartree model where  $V$  is diagonal in the *position*; the general case discussed in Sec. II where  $V$  is neither diagonal in  $r$  nor in  $k$  comprises the Brueckner theory of an infinite nucleus and the Hartree theory as special cases.

The energy of a cubic centimeter<sup>29</sup> of nuclear matter is

$$(2\pi)^{-3} \int 4\pi k^2 [\frac{1}{2}V(k) + k^2/2M], \quad (9.3)$$

<sup>29</sup> It is more convenient to calculate immediately energies per unit volume or per particle than to calculate first the total energy and then express the result in terms of the total number of particles.

where the factor  $\frac{1}{2}$  in the first term arises again from the need of counting each pair of interacting nucleons only once, while the factor 4 in front comes from the fact that for each momentum state  $\mathbf{k}$  there are four nucleons, of two spin directions and two charge values.

The determination of  $V(k)$  is the only problem of self-consistency which is treated by Brueckner *et al.* In fact, Brueckner<sup>12</sup> has pointed out that this may be a rather tedious problem because the value of  $V(k)$  is required in the second term of (3.1) or (9.10), and this second term may be large and, with Brueckner's procedure, is indeed large. Fortunately, however, this second term is greatly reduced if the exclusion principle is taken into account immediately (see Sec. X) in its evaluation (which Brueckner does not do), and in this case a very rough initial choice for  $V(k)$  will suffice for the calculation of the second term in (3.1).

We shall use for the nucleons plane-wave functions normalized to unit density. Then, if the interaction  $v_{ij}(r_{ij})$  is an ordinary potential, its matrix elements for one-nucleon functions are<sup>20</sup>

$$\begin{aligned} \langle \mathbf{k}_i' \mathbf{k}_j' | v_{ij}(r) | \mathbf{k}_i \mathbf{k}_j \rangle_P \\ = w_{ij}(\mathbf{k}_i - \mathbf{k}_i') (2\pi)^3 \delta(\mathbf{k}_i' + \mathbf{k}_j' - \mathbf{k}_i - \mathbf{k}_j), \end{aligned} \quad (9.4)$$

where  $\delta$  is the 3-dimensional  $\delta$  function and

$$w_{ij}(q) = \int v_{ij}(r_{ij}) e^{iq \cdot r_{ij}} d^3 r_{ij} \quad (9.5)$$

is the Fourier transform of the nucleon interaction. If we use a Serber force (8.20), then the matrix element of  $v_{ij}$  for the nucleus is given by (8.21) which becomes in our case

$$\begin{aligned} \langle \mathbf{k}_i' \mathbf{k}_j' | v_{ij} | \mathbf{k}_i \mathbf{k}_j \rangle_N = \frac{1}{2} [w_{ij}(\mathbf{k}_i - \mathbf{k}_i') + w_{ij}(\mathbf{k}_i - \mathbf{k}_j')] \\ \times (2\pi)^3 \delta(\mathbf{k}_i' + \mathbf{k}_j' - \mathbf{k}_i - \mathbf{k}_j). \end{aligned} \quad (9.6)$$

In the second (exchange) term, the nucleon  $i$  goes into the final state  $\mathbf{k}_j'$  and *vice versa*.<sup>21</sup>

The Eq. (3.1) determining the scattering matrix  $G$  becomes now an integral equation<sup>22</sup>:

<sup>20</sup> The factor  $(2\pi)^3$  in (9.4) and further equations is most easily understood as follows: If the momentum components of the momenta  $\mathbf{k}_i$ ,  $\mathbf{k}_j$ ,  $\mathbf{k}_i'$ ,  $\mathbf{k}_j'$  are considered quantized in a large volume, then momentum conservation permits exactly one quantized momentum state for  $\mathbf{k}_i'$  if  $\mathbf{k}_i$ ,  $\mathbf{k}_j$ , and  $\mathbf{k}_j'$  are given, and for this one state the matrix element is  $w$ , Eq. (9.5). In the continuum treatment, we have to integrate over  $\mathbf{k}_i'$  momentum space with the volume element  $(2\pi)^3 d^3 k_i'$ ; if then the integrand is Eq. (9.4), the integration yields (9.5).

<sup>21</sup> Brueckner, in reference 15, erroneously takes the final state to be  $-\mathbf{k}_i'$  which is correct only if the center of mass of the two nucleons is at rest.

<sup>22</sup> The integral in (9.7) goes only *once* over each momentum space  $\mathbf{k}_i''$ ,  $\mathbf{k}_j''$  and does not contain factors 4 for spin and charge. This is because the spin-charge function of the two nucleons in the intermediate state  $\mathbf{k}_i'' \mathbf{k}_j''$  is completely determined, *viz.*, it is the same as in the initial state  $\mathbf{k}_i \mathbf{k}_j$ , and in the final state  $\mathbf{k}_i'' \mathbf{k}_j''$ , as was shown in Sec. VIII.

$$\begin{aligned} & \langle \mathbf{k}_i' \mathbf{k}_j' | G_{ij} | \mathbf{k}_i \mathbf{k}_j \rangle \\ &= \langle \mathbf{k}_i' \mathbf{k}_j' | v_{ij} | \mathbf{k}_i \mathbf{k}_j \rangle_N - (2\pi)^{-3} \int d^3 k_i'' \\ & \quad \times d^3 k_j'' \langle \mathbf{k}_i' \mathbf{k}_j' | v_{ij} | \mathbf{k}_i'' \mathbf{k}_j'' \rangle_N \\ & \quad \times \frac{1}{E(\mathbf{k}_i'') + E(\mathbf{k}_j'') - E(\mathbf{k}_i^0) - E(\mathbf{k}_j^0)} \\ & \quad \times \langle \mathbf{k}_i'' \mathbf{k}_j'' | G_{ij} | \mathbf{k}_i \mathbf{k}_j \rangle, \end{aligned} \quad (9.7)$$

where  $\mathbf{k}_i^0$  and  $\mathbf{k}_j^0$  denote the states occupied by nucleons  $i$  and  $j$  in the chosen configuration. In (9.7) and the following, we are making the very essential simplification of assuming that (3.8) is valid for the energy of the intermediate state. We thus disregard the complications which were extensively discussed in Sec. III, *viz.*, that the scattering matrix  $G_{ij}$  and the energy of excited states  $E(\mathbf{k}_i)$  depend on the empty states and on other excited nucleons which may be present. The influence of this simplification will be briefly discussed in Sec. X. Since each matrix element of  $v_{ij}$  contains a  $\delta$  function expressing conservation of momentum, we write

$$\begin{aligned} & \langle \mathbf{k}_i' \mathbf{k}_j' | v_{ij} | \mathbf{k}_i \mathbf{k}_j \rangle_N \\ &= \langle \mathbf{k}_i' | \tilde{v}_{ij} | \mathbf{k}_i \mathbf{k}_j \rangle_N (2\pi)^3 \delta(\mathbf{k}_i' + \mathbf{k}_j' - \mathbf{k}_i - \mathbf{k}_j), \end{aligned} \quad (9.8)$$

$$\begin{aligned} & \langle \mathbf{k}_i' \mathbf{k}_j' | G_{ij} | \mathbf{k}_i \mathbf{k}_j \rangle_N \\ &= \langle \mathbf{k}_i' | \tilde{G}_{ij} | \mathbf{k}_i \mathbf{k}_j \rangle_N (2\pi)^3 \delta(\mathbf{k}_i' + \mathbf{k}_j' - \mathbf{k}_i - \mathbf{k}_j), \end{aligned} \quad (9.9)$$

and obtain the integral equation

$$\begin{aligned} & \langle \mathbf{k}_i' \mathbf{k}_j' | \tilde{G}_{ij} | \mathbf{k}_i \mathbf{k}_j \rangle \\ &= \langle \mathbf{k}_i' \mathbf{k}_j' | \tilde{v}_{ij} | \mathbf{k}_i \mathbf{k}_j \rangle_N - (2\pi)^{-3} \int d^3 k_i'' \\ & \quad \times \langle \mathbf{k}_i' \mathbf{k}_j' | \tilde{v}_{ij} | \mathbf{k}_i'' \mathbf{k}_j'' \rangle_N \\ & \quad \times \frac{P}{E(\mathbf{k}_i'') + E(\mathbf{k}_j'') - E(\mathbf{k}_i^0) - E(\mathbf{k}_j^0)} \\ & \quad \times \langle \mathbf{k}_i'' \mathbf{k}_j'' | \tilde{G}_{ij} | \mathbf{k}_i \mathbf{k}_j \rangle, \end{aligned} \quad (9.10)$$

where of course  $\mathbf{k}_i''$  and  $\mathbf{k}_j''$  are defined by momentum conservation, and  $P$  means the principal part.

In Sec. III we have shown that the intermediate states  $\mathbf{k}_i'' \mathbf{k}_j''$  must be different from all the states occupied by other nucleons,  $\mathbf{k}_i^0$ . Further, since the principal value of the integral is to be taken, they cannot both be equal to the chosen states  $\mathbf{k}_i^0 \mathbf{k}_j^0$  but at least one of them must represent an unoccupied state. Now momentum conservation requires that if  $\mathbf{k}_i'' \neq \mathbf{k}_i$ , then also  $\mathbf{k}_j'' \neq \mathbf{k}_j$ ; so at least if  $i$  and  $j$  are initially in the chosen states ( $\mathbf{k}_i = \mathbf{k}_i^0$  and  $\mathbf{k}_j = \mathbf{k}_j^0$ ), then both  $\mathbf{k}_i''$  and  $\mathbf{k}_j''$  must be unoccupied states. Hence, with plane wave functions, we may simply use the principal value  $P$  of the integral, and we do not need to use the more restrictive operator  $Q$  of Sec. III.

As we have just shown, the integral in (9.10) extends over all states in which both  $\mathbf{k}_i''$  and  $\mathbf{k}_i''' = \mathbf{k}_i + \mathbf{k}_F - \mathbf{k}_i''$  are greater than  $\mathbf{k}_F$ , the radius of the Fermi sphere. The value of  $k_F$  is given by

$$(2\pi)^{-3} 4(4\pi/3) k_F^3 (4\pi/3) r_0^3 = 1, \quad (9.11)$$

where  $r_0$  is the radius of the sphere containing one nucleon. The most accurate information on  $r_0$  for actual nuclei comes from the Stanford electron scattering experiments<sup>33</sup> and gives (for Au for which experiments and analysis are best)

$$r_0 = (1.180 \pm 0.012) \times 10^{-13} \text{ cm}. \quad (9.12)$$

Equation (9.11) yields

$$k_F = 3^{2/3} \pi^{1/3} / 2r_0 = 1.524 / r_0 = 1.29 \times 10^{13} \text{ cm}^{-1}. \quad (9.13)$$

The potential energy  $V$  defined in (9.2) is now

$$V(k_i) = 3(2\pi)^{-3} \int_0^{k_F} d^3 k_j \langle \mathbf{k}_i \mathbf{k}_j | \tilde{G}_{ij} | \mathbf{k}_i \mathbf{k}_j \rangle, \quad (9.14)$$

i.e., the integral over the diagonal elements of the reaction matrix  $G$ . As was explained in Sec. VIII, the factor 3 takes into account the fact that nucleon  $i$  interacts with the three nucleons of momentum  $\mathbf{k}_j$  which differ from it in either spin or charge. It may be noted that  $Mv_{12}(r_{12})$  is of dimension (length) $^{-2}$ ; for the Fourier transform defined in (9.5) we have  $Mw_{12}(q) \sim (\text{length})^{+1}$ , and we shall see later (Sec. XI) that  $Mw_{12}$  is related to the effective range of the potential; the  $\tilde{G}$  matrix elements are of the same dimensions as  $w$ , and  $V(k)$  according to (9.14) is again of the dimension of a potential, i.e.  $MV \sim \text{length}^{-2}$ .

The potential energy  $V(k)$ , and therefore the total energy of one nucleon  $E(k) = V(k) + k^2/2M$ , will depend on the radius of the Fermi sphere in momentum space,  $k_F$ , in addition to its dependence on  $k$ . Similarly, the interaction between two nucleons,  $\langle \mathbf{k}_i \mathbf{k}_j | \tilde{G}_{ij} | \mathbf{k}_i \mathbf{k}_j \rangle$ , will depend on  $k_F$ , because the integral in (9.10) extends over the momentum space outside the Fermi spheres  $\mathbf{k}_i'' = \mathbf{k}_F$  and  $\mathbf{k}_i''' = \mathbf{k}_F$ . If  $\tilde{G}$  were replaced by  $\tilde{v}$ , this quantity would no longer depend on  $k_F$ , but the potential energy  $V(k)$ , Eq. (9.14), would of course still do so.

The total energy of a nucleus containing  $A$  nucleons is,<sup>34</sup> according to (5.5),

$$W_{\text{tot}} = AW = \Omega \times 4(2\pi)^{-3} \int_0^{k_F} d^3 k \left[ \frac{1}{2} V(k) + \frac{k^2}{2M} \right], \quad (9.15)$$

where  $\Omega$  is the volume of the nucleus.<sup>35</sup> This clearly depends on the density of nuclear matter,

$$\rho = A/\Omega = (3/4\pi)r_0^{-3} = (2/3\pi^2)k_F^3, \quad (9.16)$$

<sup>33</sup> Hahn, Ravenhall, and Hofstadter, Phys. Rev. 101, 1131 (1956), where references to the earlier literature are also given.

<sup>34</sup> This time the sum goes over all nucleons regardless of spin, and hence there is simply a factor 4.

<sup>35</sup> One should avoid calling the volume of the nucleus  $v$  or  $V$  because this would be confused with the interaction or the potential.

and may be calculated as a function of  $\rho$ . However, as was pointed out by Eden<sup>19,20</sup> (see also Sec. II of this paper), we have not yet taken into account the requirement that the wave functions and the potential  $V$  be self-consistent. This requirement cannot easily be formulated for an infinite nucleus but this can be done for one which is extremely large. The proper procedure would of course be to choose a potential matrix  $(\mathbf{r}'|V|\mathbf{r})$ , calculate the wave functions  $\psi_n(\mathbf{r})$ , reconstruct  $V$  from this, etc., until a self-consistent solution is found. This would clearly be very difficult, and furthermore, since the nucleus is very large, it is clear physically that the exact dependence of  $(\mathbf{r}'|V|\mathbf{r})$  on the positions of  $\mathbf{r}$  and  $\mathbf{r}'$  within the boundary layer will have a negligible influence on the wave functions and the energy of the nucleus, because it will affect only the surface energy. Obviously, the only parameter in  $V$  which will seriously influence the nuclear energy is the over-all dimension of the potential well, i.e., the size of the nucleus for a given number  $A$  of nucleons. A problem of this type, where self-consistency depends almost entirely on the choice of one parameter, is eminently adapted to the variational method. Indeed, Eden<sup>19,20</sup> has shown that the self-consistent field problem in this case is equivalent to the variational problem of making the total energy a minimum as a function of the density  $\rho$ .

Thus, while it is formally possible to calculate the  $V(k)$  and the total energy for an arbitrary density, the result would in general not approximate the self-consistent solution for a large but finite nucleus. Only if the total energy is made a minimum as a function of density, will a self-consistent solution be obtained. The "solutions" for other densities may thus be considered as spurious, but they are of course useful for obtaining such quantities as the compressibility of nuclear matter, etc.

The variational condition may be rewritten

$$W = \int d^3 k \left[ \frac{1}{2} V(k) + \frac{k^2}{2M} \right] / \int d^3 k, \quad (9.17)$$

$$\frac{dW}{d\rho} = \frac{dW/dk_F}{dp} = 0. \quad (9.18)$$

Since  $W$  is a function of density only, the extra energy added when another nucleon is added to a large nucleus and the density kept constant, is given by  $W$ ; in other words, the binding energy is  $-W = |W|$ . Also if the volume is kept constant, the extra energy is  $W$  by virtue of (9.18); we have

$$\left( \frac{\partial W_{\text{tot}}}{\partial A} \right)_V = W + A \left( \frac{\partial W}{\partial A} \right)_V = W + \rho \frac{dW}{dp} = W. \quad (9.19)$$

Another way of calculating the binding energy of an extra nucleon is to consider the energy per unit volume,  $W_{\text{vol}}$ , and differentiate it with respect to the density,

i.e., effectively  $k_F$ . We have

$$\begin{aligned} \left( \frac{\partial W_{\text{tot}}}{\partial A} \right)_a &= \Omega \left( \frac{\partial W_{\text{vol}}}{\partial A} \right)_a = \frac{dW_{\text{vol}}}{d\rho} \\ &= \frac{\pi^2}{2k_F^2} \frac{d}{dk_F} \frac{1}{2\pi^3} \int d^3k \left[ \frac{1}{2} V(k) + \frac{k^2}{2M} \right], \end{aligned} \quad (9.20)$$

using (9.16). Inserting (9.14), this becomes

$$\begin{aligned} \left( \frac{\partial W_{\text{tot}}}{\partial A} \right)_a &= \frac{1}{k_F^2 dk_F} \left[ \int k^2 dk \frac{k^2}{2M} + \frac{3}{4} \frac{1}{16\pi^4} \right. \\ &\quad \times \left. \int \int d^3k_1 d^3k_2 \langle \mathbf{k}_1 \mathbf{k}_2 | \tilde{G}_{ij} | \mathbf{k}_1 \mathbf{k}_2 \rangle \right]. \end{aligned} \quad (9.21)$$

The first term, the kinetic energy, gives

$$k_F^2/2M, \quad (9.22)$$

i.e., the kinetic energy of the fastest nucleon. The second term gives three contributions: (a) from differentiation with respect to the upper limit of the  $k_1$  integral, (b) from the same for  $k_2$ , and, (c) from the dependence of  $\tilde{G}_{ij}$  on  $k_F$  arising from the solution of (9.10). We shall disregard contribution (c); this will be shown (Sec. X) to be a good approximation for normal or higher density. The contributions (a) and (b) are equal, and the factor 2 arising from this cancels the factor  $\frac{1}{2}$  with  $V$  in (9.15). Since the volume element in  $k_1$  space is  $4\pi k_1^2 dk_1$ , twice the contribution of (a) is

$$\frac{3 \times 4\pi}{4} \frac{k_F^2}{16\pi^4} \int d^3k_2 (k_F k_2 | \tilde{G}_{ij} | k_F k_2) = V(k_F), \quad (9.23)$$

if we use (9.14). Together with (9.22), we have then

$$\frac{\partial W_{\text{tot}}}{\partial A} = V(k_F) + \frac{k_F^2}{2M}. \quad (9.24)$$

This is the total one-nucleon energy of the most energetic nucleon, so that we obtain

$$W = E(k_F). \quad (9.25)$$

Thus, if (c) can be neglected, one may either use the eigenvalue of the most energetic nucleon  $E(k_F)$ , or the average energy  $W$  from (9.17).

It is perhaps somewhat surprising that one calculates in one case an average energy and in the other case a maximum energy, and that these two should be equal. This is made possible by the factor  $\frac{1}{2}$  in the potential energy when the average  $W$  is calculated in (9.17); this should just compensate for the difference between average and maximum. This argument shows, of course, that the energy of the top of the Fermi distribution,  $E(k_F)$ , must be negative. The relation (9.25) is only true if the nuclear density is chosen so as to make  $W$  a minimum; otherwise,  $W$  does not represent the energy of an additional nucleon, added at constant volume, as

can be seen from (9.19). On the other hand, this energy is correctly given by  $E(k_F)$  provided the above-mentioned contribution (c) is negligible.

## X. EXCLUSION PRINCIPLE

We shall now try to solve the integral equation (9.10) for the scattering matrix  $\tilde{G}_{ij}$ . Contrary to the procedure of Brueckner,<sup>12</sup> we shall take the Pauli exclusion principle into account from the beginning. It will be shown that this makes a large difference to the solution, and further, that the solution becomes easier rather than more difficult by taking the Pauli principle into account.

For simplicity, we shall consider the case<sup>13</sup>:

$$\mathbf{k}_i = -\mathbf{k}_i. \quad (10.1)$$

By momentum conservation in (9.10), we then have also

$$\mathbf{k}_i' + \mathbf{k}_j' = \mathbf{k}_i'' + \mathbf{k}_j'' = 0. \quad (10.2)$$

The last of these relations brings the simplification that if  $k_i'' > k_F$ , then also  $k_j'' > k_F$ , so that the allowed (unoccupied) states in the integral (9.10) all lie outside the sphere  $k'' = k_F$ , and

$$E(\mathbf{k}_i + \mathbf{k}_j - \mathbf{k}_i'') = E(k_j'') > E_F, \quad (10.3)$$

$$E(k_j) = E(k_i) < E_F. \quad (10.4)$$

The solution is best illustrated by an example. We take  $v_{ij}(r)$  to be a Yukawa interaction, which we write in terms of the effective range theory<sup>17</sup> in the form<sup>18</sup>

$$Mv_{ij} = -\frac{3.56s}{br} e^{-r/b}, \quad (10.5)$$

where  $b$  is the intrinsic range which we choose to be  $2.5 \times 10^{-13}$  cm, and  $s$  is the strength parameter. We choose  $s=1$ , which means that the scattering length for the two-body system at zero energy is infinite, corresponding to exact resonance at zero energy.<sup>19</sup> It will be convenient to introduce

$$a = b/2.12 = 1.19 \times 10^{-13} \text{ cm}; \quad (10.6)$$

then

$$Mv_{ij} = \frac{1.68}{ar} e^{-r/a}. \quad (10.7)$$

The Fourier transform (9.5) of (10.7) is

$$Mw_{ij}(q) = 4\pi \times 1.68 \frac{a}{1 + (qa)^2}. \quad (10.8)$$

For small  $q$ , this is proportional to the range  $a$  of the Yukawa potential. The potential matrix for a Serber

<sup>12</sup> The more general case,  $\mathbf{k}_i + \mathbf{k}_j \neq 0$ , is at present being considered by Mr. Thouless of the Cavendish Laboratory, Cambridge.

<sup>13</sup> It is a great advantage to use this theory so that one may be sure that all parameters are chosen consistently, in agreement with each other and with the evidence from two-body experiments.

<sup>14</sup> J. M. Blatt and J. D. Jackson, Phys. Rev. 76, 18 (1949), especially Eq. (4.4).

<sup>15</sup> Actually, a slightly greater value of  $s$  would be better since we have to take the average of singlet and triplet interaction.

force becomes, when we use (9.6), (9.8), and (10.2):

$$\langle \mathbf{k}_i' | \mathbf{k}_j' | M\tilde{v}_{ij} | \mathbf{k}_i \mathbf{k}_j \rangle_N = 2\pi \times 1.68a \left[ \frac{1}{1+a^2(\mathbf{k}_i - \mathbf{k}_j)^2} + \frac{1}{1+a^2(\mathbf{k}_i - \mathbf{k}_j')^2} \right]. \quad (10.9)$$

For the energies we use the same approximation as Brueckner,

$$E(k) = k^2/2M^*, \quad (10.10)$$

where the "effective mass"  $M^*$  is to be determined by the condition of self-consistency, and we introduce the new notation

$$v' = -M(\tilde{v}_{ij})_N, \quad G' = -M\tilde{G}_{ij}, \quad (10.11)$$

so that these quantities are now positive. We further drop the reference to the state of particle  $j$  which is given by (10.2) and the subscript  $i$  in  $\mathbf{k}_i$ , etc. Then (9.10) becomes

$$\langle \mathbf{k}' | G' | \mathbf{k} \rangle = \langle \mathbf{k}' | v' | \mathbf{k} \rangle + (2\pi)^{-3}(M^*/M) \times \int_{k_F} d^3k'' \langle \mathbf{k}' | v' | \mathbf{k}'' \rangle \frac{1}{k''^2 - k^2} \langle \mathbf{k}'' | G' | \mathbf{k} \rangle. \quad (10.12)$$

This is very similar to Brueckner,<sup>12</sup> Eq. (7), except for the lower limit  $k_F$  on  $k''$ . To start with, we shall now make the further simplifying assumption that  $k=0$ ; then the two terms in (10.9) will become equal.

We shall now show that the integral in (10.12) is numerically rather small compared with the first term on the right-hand side of (10.12). To show this, we shall use an iteration procedure: We assume that  $G'=v'$  in first approximation, we insert this into the integral and evaluate it, and then show that indeed the result is small. We calculate in particular the diagonal term

$$\langle \mathbf{k} | G' | \mathbf{k}=0 \rangle = 1.68 \times 4\pi a \left[ 1 + (2\pi)^{-3}(1.68)(4\pi a) \times \frac{M^*}{M} \times 4\pi \int_{k_F}^{\infty} \frac{k''^2 dk''}{k''^2} \frac{1}{(1+k''^2 a^2)^2} \right]. \quad (10.13)$$

The integral can easily be evaluated as a function of

$$\alpha = k_F a = 1.29 \times 1.19 = 1.53, \quad (10.14)$$

(see 9.12, 10.6), and the result is

$$\frac{\langle \mathbf{k} | G' | \mathbf{k}=0 \rangle}{\langle \mathbf{k} | v' | \mathbf{k}=0 \rangle} = 1 + \frac{2}{\pi} \frac{M^*}{M} \frac{1}{2} \left( \arctan \frac{1}{\alpha} - \frac{\alpha}{1+\alpha^2} \right) = 1 + 0.064 M^*/M. \quad (10.15)$$

Thus even if  $M^*=M$ , the integral is only about 6% of the first-order term,  $\langle \mathbf{k} | v' | \mathbf{k} \rangle$ .

This means that the Born approximation is well justified, a most remarkable result. The reason for this result is of course the exclusion principle, which greatly reduced the value of the integral. Indeed, this effect of the exclusion principle arises from the same circumstances as the rapid convergence of Brueckner's "linked cluster" expansion,<sup>13</sup> namely the fact that the matrix elements of the two-body interaction for momentum

changes of the order of  $k_F$  are small. The small result for the second term in (10.15) justifies, of course, the use of the iteration procedure for solving (10.12). It further justifies the use of the rough approximation (10.10) for the energy in the denominator.

It is easy to see that the contribution of the second term in (10.15) would be even smaller if the density had been chosen higher. This would give a large value of  $k_F$  and of  $\alpha$ , and in this limit the term in parentheses in (10.15) becomes  $2/(3\alpha^3)$ , and

$$\frac{\langle \mathbf{k} | G' | \mathbf{k}=0 \rangle}{\langle \mathbf{k} | v' | \mathbf{k}=0 \rangle} = 1 + 0.36 \alpha^{-3} \frac{M^*}{M}. \quad (10.16)$$

The contribution thus decreases inversely as the density of the nucleus, and the Born approximation becomes increasingly good at high density because the Pauli principle takes more and more effect.<sup>14</sup>

On the other hand, if the exclusion principle had not been taken into account,  $k_F$  would have to be replaced by zero. Then  $\alpha$  in (10.14) is zero, and (10.15) is replaced by

$$1 + 0.84 M^*/M. \quad (10.17)$$

In this case, the deviation from Born approximation is large, and the iteration procedure is no longer applicable. This is the case treated by Brueckner,<sup>12</sup> and in this case it is necessary to solve the integral equation (10.12) explicitly, instead of simply carrying out a quadrature. Brueckner was able, in his case, to reduce the integral equation to a differential equation in coordinate space, a reduction which becomes more complicated if the Pauli principle is taken into account.<sup>15</sup> However, a differential equation is still more complicated than a quadrature, so that the exclusion principle still remains a simplification.

It might be argued<sup>16</sup> that a good approximation could still be obtained by solving Eq. (10.12) without taking the Pauli principle into account. Indeed, we have shown that a good approximation to (10.12) is obtained if  $G'$  in the integral is replaced by  $v'$  and then the Pauli principle is taken into account. The total potential energy of the nucleus is then proportional to

$$\begin{aligned} & \int d^3k_i d^3k_j \langle \mathbf{k}_i \mathbf{k}_j | \tilde{G} | \mathbf{k}_i \mathbf{k}_j \rangle \\ &= \int d^3k_i d^3k_j \langle \mathbf{k}_i \mathbf{k}_j | \tilde{v} | \mathbf{k}_i \mathbf{k}_j \rangle \\ &+ (2\pi)^{-3} \int d^3k_i d^3k_j d^3k_i' d^3k_j' \langle \mathbf{k}_i \mathbf{k}_j | \tilde{v} | \mathbf{k}_i' \mathbf{k}_j' \rangle |^2 \\ & \times \frac{\delta(\mathbf{k}_i' + \mathbf{k}_j' - \mathbf{k}_i - \mathbf{k}_j)}{E_i'' + E_j'' - E_i - E_j}, \end{aligned} \quad (10.18)$$

<sup>12</sup> The same conclusion has been reached by W. J. Swiatecki. Starting from perturbation theory and taking into account the exclusion principle, he finds that the Born approximation is quite good at the observed nuclear density while it would be very poor at low density. I am indebted to Dr. Swiatecki for sending me his manuscript before publication.

<sup>13</sup> See, e.g., Brueckner, reference 12, footnote 5.

where the integral over  $k_i''$  and  $k_j''$  goes only over unoccupied states. Now, in this form, nothing would be changed if the integral over  $k_i''$  and  $k_j''$ , were extended also over occupied states, because interchange of the integration variables  $k_i''k_j''$  with  $k_ik_j$  would give the same contribution with opposite sign. However, three things are wrong with this argument. First, the energies in the denominator in (10.18) will be different according to whether the Pauli principle is taken into account or not, so that the contribution of the unoccupied states  $k_i''k_j''$  will be different in the two cases (it will be less when the Pauli principle is not taken into account because the effective mass will then be lower). Secondly, while the first iteration provides a good solution of (10.12) when the Pauli principle is taken into account, this is not so when it is disregarded [see Eq. (10.17)]. In this latter case, then, there is no reason for (10.18) to be a good approximation to the energy of the nucleus. Third, the interchange of integration variables is only possible if both  $k_i''$  and  $k_j''$  are occupied. A large contribution comes from  $k_i''$  occupied,  $k_j''$  empty or *vice versa*, and this is not compensated by interchange of initial and intermediate states.

The small contribution of the integral in (10.12) has been demonstrated only for the case  $k=0$ . For  $k \neq 0$ , the denominator  $k''^2 - k^2$  in (10.12) becomes smaller. However, crude estimates show that the increase of importance of the second term in (10.12) with  $k$  is very slow, and only when  $k$  is very close to  $k_F$  does it become appreciable. Mr. Thouless of Cambridge University has done quantitative calculations which show that the correction to the potential energy of a particle remains small even near  $k_F$ , although it is then of course larger than for  $k=0$ .

In correspondence with K. A. Brueckner, the following interesting comparison has been developed between the solution with and without exclusion principle (EP). According to (10.18), the *average* value of the second term in the iteration expansion of  $G$  is the same in both solutions [disregard the third argument given below Eq. (10.18)]. From (10.15) and (10.17), we know that for  $k=0$  this second term is larger without EP, leading to a lowering of the energy level  $k=0$ . For  $k=k_F$ , the reverse must then be the case, i.e., the energy level lies higher without the EP than with it. [Indeed, in some cases, the highest occupied level calculated without EP turned out to lie above zero energy, which is incompatible with Eq. (9.25).] Generally, it follows that the

nucleon levels calculated without EP will be too much spread out in energy; in other words, that the effective mass will turn out too low. This in turn will reduce the value of the second iterated term in  $G$  and thus the error made by neglecting the EP. The error in the average binding energy due to neglect of EP should be less than in the effective mass.

Our method of solution of (10.12) holds of course only for "well-behaved" interactions  $v_{ij}(r)$ , such as the "classical" shapes Yukawa, exponential, Gaussian, and square well. It obviously cannot hold if the interaction contains a repulsive core, because in this case the Fourier transform (6.5) of the potential is infinite (and repulsive). The integral equations (9.10) and (10.12) are still alright if  $v$  is interpreted as the limit of a finite repulsive core. But the solution by iteration becomes meaningless; therefore Brueckner *et al.*, who were mostly interested in repulsive-core potentials, could not make use of our iteration procedure. Instead, it is necessary to transform the equations (9.10) and (9.12) back to coordinate space. In this form, the equations are more complicated with the exclusion principle than without, and it is therefore natural that Brueckner in his first solution<sup>12</sup> neglected the EP.

A solution of the problem of a pure repulsive core with Pauli principle has been obtained by Bethe and Goldstone,<sup>23</sup> using a suitable coordinate space equation. Brueckner (private communication) has obtained a numerical solution for a more realistic case, *viz.*, a deep and narrow attractive well outside a repulsive core, and has found that in this case the effect of the exclusion principle is not large.

Finally, we want to consider briefly the complications discussed in Sec. III. These can easily be taken into account if the integral equations can be solved by iteration, as seems to be the case for our simple potentials. We may as a first approximation set  $G_{ij}=v_{ij}$ , obtain the potential energy  $V(k)$  from (9.14), and set  $E(k)=k^2/2M+V(k)$ , for all  $k$ . Then, in second approximation, we set  $G_{ij}=v_{ij}$  under the integral in (9.10)—as we did in solving (10.12)—and insert the just-obtained values of  $E(k)$  in the denominator of (9.10). To this approximation, the complications of Sec. III have no influence on the reaction matrix and on the energy of a nucleon in the chosen configuration. Now we use the same (second) approximation to calculate the reaction matrix for an excited state; according to (3.7), we get, with the notation of (10.12):

$$(k'_i k'_j | G_{ii'} | k_i k_i^0; k_j^0 k_j^0, k_j) = (k'_i k'_j | v_{ii'} | k_i k_i^0)_N + (2\pi)^{-3} \int d^3 k_i'' (k'_i k'_j | v_{ii'} | k_i'' k_i'')_N \\ \times \frac{M}{E(k_i'') + E(k_i + k_i^0 - k_i'') + E(k_j) - E(k_i^0) - E(k_j^0) - E(k_j^0)} (k'_i k'_j | v_{ii'} | k_i k_i^0)_N. \quad (10.19)$$

The diagonal elements of this matrix,

$$\langle \mathbf{k}, \mathbf{k}_i^0 | G_{ii'} | \mathbf{k}, \mathbf{k}_i^0; \mathbf{k}, \mathbf{k}_{i'}^0, \mathbf{k}, \mathbf{k}_j^0 \rangle,$$

are then inserted into (3.5) to give the (second approximation to) the energy of the state in which nucleons  $i$  and  $j$  are excited. Since the second term of (10.19) will again be a few (maybe 3)<sup>42</sup> percent of the first, its dependence on the empty states  $\mathbf{k}_i^0, \mathbf{k}_j^0$  and on the extra occupied state  $\mathbf{k}$ , will be only a fraction of this amount; let us say, about one percent for the common choices of these three states. Thus in practice the energy of the state  $\mathbf{k}$ , will depend on the supernumerary quantum numbers  $\mathbf{k}_i^0, \mathbf{k}_j^0, \mathbf{k}$ , only to about 1%, and to this accuracy it is possible to define  $V(\mathbf{k}_i)$  and  $E(\mathbf{k}_i)$ . In third approximation, then, the energies of the excited states  $\mathbf{k}_i, \mathbf{k}_j$  as calculated from (10.19) can be inserted in the denominator of (9.10), and at the same time  $G$  in (9.10) replaced by the second approximation calculated in (10.15). Since the second term in (10.15) is only about 5% of the first, and the approximation of  $\delta(\mathbf{k}, \mathbf{k}_i; \mathbf{k}_i^0, \mathbf{k}_j^0)$  of (3.5) by the denominator in (9.10) is good to about 1%, the error in the energy of the ground state caused by this approximation will be about 0.05% which is completely negligible.

Thus the complications discussed in Sec. III are of no practical importance for well-behaved nucleon interactions such as the Yukawa interaction discussed in this section. However, for potentials with a repulsive core these complications may be much more important.

#### XL INTERACTION IN S STATES ONLY

For an adequate treatment of the saturation problem, it is necessary to use nuclear forces with a repulsive core. A method for solving the integral equation (9.10) with such forces and with the Pauli principle is given by Bethe and Goldstone.<sup>23</sup> However, much work will be required before reliable results can be obtained. It is therefore desirable, for a preliminary orientation, to investigate a potential which gives saturation without having a repulsive core.

Such a potential is suggested by Brueckner's paper<sup>12</sup> on the evaluation of his theory. He uses an interaction which exists only in  $S$  states, which he justifies on physical grounds.<sup>43</sup> Now such an interaction, even if it contains no repulsive core,<sup>44</sup> will always lead to saturation. This can be seen most easily by a statistical argument. A given nucleon in a large (infinite) nucleus will interact essentially with all those nucleons which are in  $S$  states with respect to the given nucleon, and are within a sphere whose radius is equal to the range of the nuclear forces,  $b$ . Thus the number of interactions

<sup>42</sup> Since the denominator in (10.19) contains three excitation energies rather than the two in (9.10), the value of the integral term in (10.19) is estimated to be only  $\frac{1}{3}$  of that in (10.12).

<sup>43</sup> If one assumes a Serber force, there is no interaction in  $P$  states.  $D$ -state interaction is small at the normal nuclear density provided there is a strong tensor force [Brueckner (private communication)].

<sup>44</sup> Brueckner's  $S$ -state interaction does contain a repulsive core.

per nucleon is proportional to the number of  $S$  states within a sphere of radius  $b$ , which in turn is proportional to  $k_F b$ . Therefore the attractive potential energy is proportional to  $k_F$  and hence to the cube root of the density. [This will be shown quantitatively in (11.17) and (11.19).] The kinetic energy is proportional to  $k_F^2$ . The combination of two such terms clearly leads to a minimum of the total energy at some definite value of  $k_F$  and hence to saturation. The difference from the case of an ordinary or a Serber force is, of course, that in these latter two cases the potential energy per nucleon is proportional to the density, and thus to  $k_F^3$ , so that no minimum of the total energy exists.

Interaction in  $S$  states only does, of course, not correspond to an ordinary potential, but we may speak of the potential acting between two nucleons in an  $S$  state and denote it by  $v_{ij}(r)$ . We must now derive the matrix elements  $\langle \mathbf{k}', \mathbf{k}' | v_{ij} | \mathbf{k}, \mathbf{k}_i \rangle_P$ . It is convenient to use center-of-mass coordinates so that  $\mathbf{k}_i = -\mathbf{k}_j$  and then to drop the subscript  $i$ . The desired matrix element is then the spherically symmetric part of the Fourier transform of  $v_{ij}(r)$ , or in other words, the average of the Fourier transform over all directions of the final momentum  $\mathbf{k}'$ , keeping the direction of the incident wave fixed. Thus we have, using a notation similar to (9.8) and (9.5):

$$\langle \mathbf{k}' | v_{ij} | \mathbf{k} \rangle_P = \int \frac{d\omega'}{4\pi} w(\mathbf{k} - \mathbf{k}'). \quad (11.1)$$

Now  $w$  depends only on

$$q = |\mathbf{k} - \mathbf{k}'|, \quad (11.2)$$

and if  $\theta$  is the angle between  $\mathbf{k}$  and  $\mathbf{k}'$ ,

$$d\omega' = 2\pi \sin\theta d\theta = 2\pi q dq / kk', \quad (11.3)$$

so that

$$\langle \mathbf{k}' | v_{ij} | \mathbf{k} \rangle_P = (2kk')^{-1} \int_{|\mathbf{k}-\mathbf{k}'|}^{k+k'} q d\omega' w(q). \quad (11.4)$$

Since the  $S$  state has even parity, exactly the same result will be obtained if the forces are Majorana exchange or Serber forces.

The integral in (11.4) gives a slightly simpler result if we use an exponential potential rather than the Yukawa interaction between two nucleons. Again using the effective range formula of Blatt and Jackson,<sup>25</sup> Eq. (4.4), we have

$$Mv_{ij}(r) = -\frac{1.446s}{a^2} e^{-r/a}, \quad (11.5)$$

where  $a = b/3.54$ , with  $b$  the intrinsic range of Blatt and Jackson. Taking again  $b = 2.5 \times 10^{-13}$  cm, we have  $a = 0.706 \times 10^{-13}$  cm. The strength parameter  $s$  will again be set equal to one (exact resonance). Then

$$\begin{aligned} -Mw(q) &= -4\pi \int Mv_{ij}(r) r^2 dr \frac{\sin qr}{qr} \\ &= 8\pi \times 1.446a (1 + a^2 q^2)^{-2}, \end{aligned} \quad (11.6)$$

and (11.4) becomes, with the notation (10.11):

$$(k'|v'|k) = \frac{1.446 \times 8\pi a}{2kk'} \int \frac{qdq}{(1+a^2q^2)} \\ = \frac{1.446 \times 8\pi a}{[1+a^2(k-k')^2][1+a^2(k+k')^2]}. \quad (11.7)$$

Now it was shown in Sec. X that the reaction matrix  $G'$  is nearly equal to the potential matrix  $v'$ . We are then interested in the diagonal elements  $k'=k$  of  $v'$ , and we get

$$(k|v'|k) = \frac{1.446 \times 8\pi a}{1+4a^2k^2}. \quad (11.8)$$

Going back to the laboratory system, we have  $2k=k$ ,  $-k_j$ , which we shall denote by  $K$ , and

$$M(k_i/k_j|v|k_ik_j) \\ = -\frac{1.446 \times 8\pi a}{1+a^2K^2} (2\pi)^3 \delta(k_i' + k_j' - k_i - k_j). \quad (11.9)$$

The potential acting on one particle  $k_i$  is, from (9.14),

$$-MV(k_i) = -3(2\pi)^{-3} \int d^3k_j (k_i k_j | G_{ij}' | k_i k_j) \\ = \frac{1.446 \times 24\pi a}{(2\pi)^3} \frac{2\pi}{k_i} \int_0^{k_F} k_j dk_j \int_{|k_i-k_j|}^{k_i+k_j} \frac{K dK}{1+a^2K^2}. \quad (11.10)$$

This can easily be evaluated by integrating first over  $k_j$  and then over  $K$ . If we use

$$\kappa = k_i a, \quad \kappa_F = k_F a, \quad (11.11)$$

the result is

$$-MV(k_i) = \frac{1.446 \times 6}{\pi a^2} \left[ \frac{\kappa_F^2 - \kappa^2 + 1}{4\kappa} \ln \frac{1 + (\kappa_F + \kappa)}{1 + (\kappa_F - \kappa)} \right. \\ \left. + \kappa_F - \text{arc tan}(\kappa_F + \kappa) - \text{arc tan}(\kappa_F - \kappa) \right]. \quad (11.12)$$

In the limit  $\kappa=0$  we get for the expression in square brackets in (11.12)

$$[ ] = 2(\kappa_F - \text{arc tan}\kappa_F), \quad (11.13)$$

while in the limit  $\kappa=\kappa_F$  the result is

$$[ ] = \frac{1}{4\kappa_F} \ln(1+4\kappa_F^2) + \kappa_F - \text{arc tan}2\kappa_F. \quad (11.14)$$

If, in addition,  $\kappa_F$  is very small, both of these expressions reduce to  $\frac{3}{4}\kappa_F^3$  which can easily be checked directly from (11.10). In this limit (i.e., for very low density), the potential  $V$  does not depend on velocity.

For the adopted nuclear constants,  $\kappa_F = 1.29 \times 10^{-13}$

and  $a = 0.706 \times 10^{-13}$ , we have

$$\kappa_F = 0.91, \quad (11.15)$$

$$[ ] = 0.346 \quad \text{for } \kappa=0, \quad (11.16)$$

$$[ ] = 0.244 \quad \text{for } \kappa=\kappa_F.$$

Thus the potential decreases by a factor of 1.42 from the slowest to the fastest nucleon.

For very high density, we have

$$[ ] = 2(\kappa_F - \pi/2) \quad \text{for } \kappa=0, \quad (11.17)$$

$$[ ] = \kappa_F - \pi/2 \quad \text{for } \kappa=\kappa_F,$$

so that there is then a factor of 2 between slowest and fastest nucleon. As was shown in Sec. X, the assumption  $G=v$  is best in this limit.

The most interesting quantity is the *average* of the potential  $V$  over the Fermi sphere [one-half of this quantity is the average potential energy per nucleon, see Eq. (9.15)]. This is obtained by integrating first over  $k_i$  and  $k_j$  and last over  $K$ . The result is

$$-MV_\infty = -M \int_0^{k_F} V(k_i) k_i^2 dk_i / \int k_i^2 dk_i \\ = \frac{1.446 \times 6}{\pi a^2} \left[ -\frac{1}{4\kappa_F} + \frac{3}{2} + \frac{1}{\kappa_F} \left( \frac{3}{4} + \frac{1}{16\kappa_F^2} \right) \right. \\ \left. \times \ln(1+4\kappa_F^2) - 2 \text{arc tan} 2\kappa_F \right]. \quad (11.18)$$

For small  $\kappa_F$ , the expression in square brackets is of course again  $\frac{3}{4}\kappa_F^3$ . For large  $\kappa_F$ , it is

$$[11.18] = \frac{3}{2}(\kappa_F - \frac{3}{2}\pi) \quad (11.19)$$

which approaches the mean of the two values given in (11.17). For  $\kappa_F = 0.91$ , it is

$$[11.18] = 0.280 \quad (11.20)$$

closer to the lower of the two values in (11.16). [11.18] means the expression in square brackets in Eq. (11.18).

The kinetic energy of any nucleon is

$$MT = \frac{1}{2}k^2 = \frac{1}{2a^2}\kappa^2, \quad (11.21)$$

and the average kinetic energy is

$$MT_\infty = \frac{1}{2}(\frac{3}{2}\kappa_F^2) = \frac{3}{10a^2}\kappa_F^2. \quad (11.22)$$

The binding energy per nucleon is conveniently written in the form

$$W = \frac{3}{10Ma^2} \{-\kappa_F^2 + (4/3)\alpha[11.18]\}. \quad (11.23)$$

where

$$\alpha = 15 \times 1.446 / 2\pi = 3.452, \quad (11.24)$$

TABLE I. Nuclear energies at two densities in Mev (exponential interaction, no repulsive core).

1. Density:	Observed	Optimal	Optimal, $\alpha \gg 1$
2. $\kappa_F$ (in $10^{12} \text{ cm}^{-1}$ )	0.91	2.92	$\alpha \gg 1$
3. $r_0$ (in $10^{-12} \text{ cm}$ )	1.18	0.367	$1.07/\alpha^2$
4. Mean kinetic energy	20.7	213	$\alpha^2$
5. Mean potential energy (negative)	32.3	278	$2\alpha^2$
6. Mean binding energy $W$	11.6	65	$\alpha^2$
7. Slowest nucleon, binding energy	79.7	775	$(16/3)\alpha^2$
8. Fastest nucleon, negative potential energy	56.3	420	$(8/3)\alpha^2$
9. Fastest nucleon, kinetic energy	34.5	355	$(5/3)\alpha^2$
10. Fastest nucleon, negative eigenvalue	21.8	65	$\alpha^2$
11. Variation of potential energy	23.4	355	$(8/3)\alpha^2$
12. Ratio to variation of kinetic energy, $r$	0.68	1.00	1.6
13. $M^*/M$	0.595	0.500	0.384

when we recall that the average interaction energy per nucleon is one-half of the  $V_{\infty}$  given in (11.18).

If we insert for [11.18] the asymptotic value (11.19), the maximum of  $W$  occurs at

$$\kappa_F = \alpha \quad (11.25)$$

[this is the reason for the choice of the coefficient in (11.23)]. For the actual value of  $\alpha$ , 3.452, the asymptotic formula (11.19) is not accurate enough, and the minimum of (11.18) is found to occur at  $\kappa_F = 2.92$ . This value of  $\kappa_F$  is more than three times the "observed" value  $\kappa_F = 0.91$ , Eq. (11.15). In other words, inserting the actual strength of the nuclear forces and using interaction in  $S$  states only, we obtain a nuclear radius (in equilibrium) more than three times too small, a nuclear density about thirty times too large. [Using (11.25) and (11.24) would be even worse.]

In Table I, we give the numerical values of various physical quantities for  $\alpha = 3.452$  and two different values of the density, one the observed density of nuclear matter ( $\kappa_F = 0.91$ ) and the other the density which makes  $W$  in (11.18) a maximum (called "optimal density" in Table I,  $\kappa_F = 2.92$ ). All energies for these two cases are given in Mev, and the range of the exponential interaction is assumed to have the value  $a = 0.706 \times 10^{-12} \text{ cm}$ .

In the last column of Table I, we have considered yet another case of still less physical meaning, but of some mathematical interest. We have assumed that the nuclear forces are increased in strength so that  $\alpha$  is larger than (11.24). Then the asymptotic formulas (11.19) and (11.20) do become valid, and all physical quantities can be expressed in a simple manner in terms of  $\alpha$ . In this column, all energies are in units of

$$B = 3/10 M a^2, \quad (11.26)$$

which has the value 25.0 Mev for  $a = 0.706 \times 10^{-12} \text{ cm}$ .

The first three rows of the table describe the case considered. The next three give the energy of an average

nucleon, viz., its kinetic, potential, and total binding energy; in particular, line 5 is the average potential energy per nucleon, or one-half of the average of the one-particle potential  $V$ . The seventh row gives the negative eigenvalue of a nucleon of zero momentum, and the following three refer to the fastest nucleon. Of these rows, line 8 gives the negative of the one-particle potential for  $\kappa = \kappa_F$ .

Line 11 gives the change of the one-particle potential from the slowest to the fastest nucleon, and line 12 the ratio of this change to the kinetic energy of the fastest nucleon (line 9). Assuming the variation of potential energy to be quadratic in  $\kappa$ , the effective mass is then  $M^*/M = 1/(1+r)$ , and is given in the last line of the table.

We first note that, according to Sec. IX, the negative eigenvalue of the fastest nucleon (line 10) should be equal to the average binding energy  $W$  (line 6), and this is indeed true for the two last columns in which the density (i.e.,  $\kappa_F$ ) has been adjusted to make  $W$  a maximum. For the "observed" nuclear density (and the adopted values of  $a$  and  $\alpha$ ),  $W$  is not a minimum and lines 10 and 6 therefore do not agree. This case, therefore, is not a solution of the self-consistent problem (Sec. IX) and the numbers in the table for this case are actually not meaningful.

It has already been pointed out that the maximum of  $W$  occurs at a very high density. Indeed,  $\kappa_F = 2.92$  is 3.2 times larger than the "observed"  $\kappa_F$  of 0.91, and therefore the density is about 33 times too high. This shows that the assumption of interaction in  $S$  states only, while it formally gives saturation, does not give saturation at the correct density at all. It is to be hoped that the introduction of a repulsive core will improve this situation—indeed, this surely must lead to an equilibrium density far lower than corresponds to  $r_0 = 0.367$  because for this value of  $r_0$  the repulsive core from one nucleon would almost reach the next nucleon, if the conventional value  $r_0 = 0.6 \times 10^{-12} \text{ cm}$  is assumed for the radius of the core.

At the high density  $\kappa_F = 2.92$ , all energies are naturally very high. The binding energy per nucleon, 65 Mev, may be compared with the volume energy of 15.5 Mev per nucleon deduced by Green and Engler<sup>46</sup> from empirical data on nuclear binding energies. At that, the theoretical binding energy is a relatively small difference between the potential and kinetic energy, each of which is over 200 Mev for an average nucleon. The eigenvalue of the slowest nucleon is even larger, viz., almost 800 Mev. It is clear that none of these numbers have any relation to actual nuclear energies.

We now consider the results at the observed nuclear density,  $\kappa_F = 0.91$ . This is not legitimate since  $W$  is not a maximum. We could imagine, however, that an added core might change the position of the maximum of  $W$  so as to give the correct density, and might at the same

<sup>46</sup> A. E. S. Green and N. A. Engler, Phys. Rev. 91, 40 (1953).

time not change  $W$  itself very much. Assuming hopefully that this can be achieved, the binding energy  $W$  of 11.6 Mev is now in reasonable agreement with the observed value of 15.5 Mev, closer in fact than our crude assumptions about the nuclear interaction warrant. Thus there is some hope that if the theory can be made to yield the correct density, it will then also yield a good value for the binding energy.

Our model, just like Brueckner's,<sup>12</sup> gives a large increase of the one-particle potential  $V$  with momentum. This increase is quite comparable with that of the kinetic energy. Indeed, the ratio of the two (line 12) varies from 0.7 to 1.6 for the three cases considered, increasing with increasing density. For the case  $\kappa_F = 2.92$ , the ratio is accidentally exactly 1. The corresponding effective masses range from about 0.6 to 0.4. If we consider the case of the observed density as significant, even though  $W$  is not maximized, we should expect an effective mass of about 0.6 which is somewhat larger than that reported by Brueckner.<sup>12</sup>

## XII. CLUSTER TERMS

In Sec. IV it has been shown that the Brueckner method will work satisfactorily provided that certain terms, which we have called cluster terms, are small. The most important of these is the correction to the energy,

$$\Delta E = \langle \Phi_0 | \sum_{ij} I_{ij} L_{ij} | \Phi_0 \rangle = \sum_{ij} \langle I_{ij} \Phi_0, L_{ij} \Phi_0 \rangle, \quad (12.1)$$

where  $\Phi_0$  is the model wave function of the ground state, the sum goes over all pairs of nucleons, and  $L_{ij}$  includes all terms of the operator  $F_{ij}$ , Eq. (4.3), which are "linked" to the pair  $ij$ . Another interesting quantity is  $\Delta E_i$ , which is the contribution to (12.1) from clusters which involve one particular particle  $i$ . If the chosen configuration is degenerate, we shall be interested in the matrix elements of  $\sum_i I_{ij} L_{ij}$  between two degenerate configurations; these will be considered in Sec. XVI. In the present section, we shall evaluate the cluster term of Eq. (12.1).

It was shown in (7.2) and (7.8) that the only non-vanishing matrix elements of  $I_{ij}$  starting from the chosen configuration  $C$  are those in which both nucleons  $i$  and  $j$  become excited. Hence  $I_{ij} \Phi_0$  contains only such model states in which  $i$  and  $j$  are excited while all other nucleons are in their chosen states.  $L_{ij}$  of Sec. IV may be expanded thus:

$$L_{ij} = 1 + \sum_{i \neq j} \frac{Q}{e_{ii}} I_{ii} + \sum_{i \neq j} \frac{Q}{e_{jj}} I_{jj} + \sum_{i \neq j} \frac{Q}{e_{ii}} I_{ii} \sum_{m \neq i} \frac{Q}{e_{im}} I_{im} \\ + 3 \text{ other terms involving 2 factors } I \\ + \text{ terms involving 3 or more factors } I. \quad (12.2)$$

In the energy denominators  $e$ , the nucleons excited at each stage have been put in evidence. The first term inserted in  $L_{ij} \Phi_0$  of Eq. (12.1) gives  $\Phi_0$  which is clearly orthogonal to  $I_{ij} \Phi_0$ . In the second

(third) term,  $l$  must be different from  $j$  ( $i$ ), so that  $I_{il} \Phi_0 (I_{ij} \Phi_0)$  is again orthogonal to  $I_{ij} \Phi_0$ . Only the next term in (12.2) can give a nonvanishing result,

$$\Delta E_3 = \sum_{ijk} \left( \Phi_0 \left| I_{ij} \frac{Q}{e_{ii}} I_{jk} \frac{Q}{e_{kk}} I_{ki} \right| \Phi_0 \right). \quad (12.3)$$

In this term, the three nucleons  $i$ ,  $j$ , and  $k$  are successively excited. There are of course also terms in which more nucleons are successively excited and de-excited.

The term (12.3) was first derived by BL, Eq. (20). It was investigated by Brueckner<sup>15</sup> who called it a cluster term. According to Brueckner,  $\Delta E_3$  is the contribution to the energy of a cluster of three particles which interact simultaneously. When we constructed the  $G$  matrix, in Eq. (3.1) or (9.10), the influence of particles other than the two interacting particles  $i, j$  was already taken into account, but only insofar as it could be expressed as an over-all potential which influenced the excitation energies  $E(n'_i) - E(n_i)$  of the interacting particles  $i$  and  $j$ . Thus (12.3) (and higher cluster terms) are required only to take into account the fluctuations of the influence of other particles (in this case  $k$ ) on the interaction of two particles  $i$  and  $j$ . From this description it becomes plausible that  $\Delta E_3$  should be small: It is necessary that while  $i$  and  $j$  interact strongly, a third particle  $k$  be so close that it also has a much higher interaction with them than the average. This is very unlikely, no matter what the nuclear density is: If it is high, then many nucleons are always close to particles  $i$  and  $j$ , and their action can be approximated by an average. If the density is low, and if no actual clusters are formed (see, however, the discussion below), then it is geometrically very improbable that three nucleons come close enough together so that all of them interact strongly—in this case, the influence of the other particles on  $i$  and  $j$  can be omitted altogether. This argument is clearly an essential point for the success of the Brueckner method. Whether it is valid can be decided only by actual calculation of  $\Delta E_3$  and possibly higher cluster integrals.

Such an actual calculation has been carried out by Brueckner<sup>16</sup> and will be repeated in this section. Like Brueckner, we shall assume for the present that the interaction is of the Serber type, (8.20), and has the spatial dependence of a Yukawa potential, (10.5). Other possibilities will be discussed at the end of this section.

Let us assume that the nucleons  $i, j, k$  have respectively the orbitals (spatial wave functions)  $a, b, c$  in the chosen configuration. Further we assume that the interactions take place in the order  $ij, jk, ki$ , as shown in (12.3); thus the order of the three orbitals  $a, b, c$  is meaningful. Since two or even all three orbitals may be alike,  $N^3$  different choices of the orbitals  $a, b, c$  are possible if  $N = A/4$  is the total number of orbitals occupied.

We must first discuss the influence of spin and charge. Considering  $a$ ,  $b$ , and  $c$  different (the other case being unimportant), there are 64 different spin-charge combinations which may be associated with the three orbitals in the chosen configuration. We may call the three spin-charge wave functions  $\alpha, \beta, \gamma$ ; they are initially associated with  $a, b, c$ , respectively, so that the order of  $\alpha, \beta, \gamma$  is meaningful. Several cases may arise:

1. The spin-charge states  $\alpha, \beta, \gamma$  may all be different; there are 24 possible choices of  $\alpha, \beta, \gamma$  corresponding to this case. Then it can be shown (see Appendix) that in the two intermediate states the spins must be the same as in the chosen state: In the first intermediate state, the wave functions of the three nucleons are  $a'\alpha$ ,  $b'\beta$ , and  $c'\gamma$ , in the second  $a'\alpha$ ,  $b\beta$ , and  $c'\gamma$ . That is to say, we can choose the orbitals  $a', b', c'$  of the intermediate states (keeping in mind momentum conservation, however), but we have no further choice of the spins. If we disregard the difference between  $G'$  and  $v'$ , as is reasonable for the Yukawa interaction according to Sec. X, then each matrix element  $I_{ij}$ ,  $I_{jk}$  and  $I_{ki}$  in (12.3) becomes the matrix element of the interaction  $v$ .

2. Two of the spin-charge states may be the same; there are 36 choices of this type. It is shown in the Appendix that for a Serber force the result is zero if either  $\alpha=\beta$  or  $\alpha=\gamma$ , and that each of the 12 states  $\beta=\gamma$  gives a contribution which is the negative of that from the states of type 1. This is due to the fact that there must be three exchanges of spin between orbitals.

3. If all three spin-charge states are the same (4 cases), the result is zero.

Thus, for a Serber force, the result is as if there were only 12 rather than 64 spin-charge states for any triple of orbitals  $a, b, c$ . This factor, reducing the result, was not taken into account of Brueckner. We also propose to omit it for the moment because (a) this facilitates comparison with Brueckner, (b) the factor depends on the special assumption of a Serber force, and (c) the negative contribution of the spin distributions of type 2 seems to depend on the fact that an odd number of interactions is involved, hence the small result for 3-particle clusters may not be repeated for the 4-particle type.

We now consider again an infinite nucleus so that the initial nucleon orbitals are defined by their momenta  $k_i$ ,  $k_j$ , and  $k_k$ . Because of momentum conservation, only one further momentum can be chosen; we take it to be the momentum change of nucleon  $j$  in the first transition and call it  $q$ . Then after the first transition we have

$$k'_i = k_i - q; \quad k'_j = k_j + q; \quad k'_k = k_k, \quad (12.4)$$

and after the second transition

$$k''_i = k_i - q; \quad k''_j = k_j; \quad k''_k = k_k + q. \quad (12.5)$$

The initial states  $k_i$ ,  $k_j$ , and  $k_k$ , which lie inside the Fermi sphere, and the momentum change  $q$ , must all

be chosen so that the intermediate states  $k'_i$ ,  $k'_j$  and  $k'_k$  lie outside the Fermi sphere.<sup>46</sup>

The energy will again be assumed to depend quadratically on  $k$ , Eq. (10.10). The Fourier transform of the potential is given by (10.8), and we shall use the abbreviation

$$f(q) \equiv f(q) = 1/[1 + (qa)^2]. \quad (12.6)$$

Then with our assumptions and notations, the three-particle cluster term gives a result similar to Brueckner's<sup>18</sup> Eqs. (59) and (62). The contribution per particle is

$$\Delta E_3/A = -(2\pi \times 1.68a)^3 (2M^*)^2 M^{-3} 64 (2\pi)^{-12}$$

$$\begin{aligned} & \times \int^{k_F} d^3 k_i \int^{k_F} d^3 k_j \int^{k_F} d^3 k_k \int d^3 q \\ & \times [f(q) + f(k_i - k_j + q)] [f(q) + f(k_k - k_j)] \\ & \times [f(q) + f(k_k - k_i + q)] [(k_i - q)^2 + (k_i + q)^2 \\ & - k_i^2 - k_j^2]^{-1} [(k_j - q)^2 + (k_k + q)^2 - k_k^2 - k_j^2]^{-1} \\ & \times \left[ 4(2\pi)^{-3} \int^{k_F} d^3 k \right]^{-1}, \end{aligned} \quad (12.7)$$

where it is understood that  $|k_i - q|$ ,  $|k_j + q|^2$  and  $|k_k + q|$  must all be greater than  $k_F$ . The use of  $2\pi$  in the first factor, rather than  $4\pi$ , takes into account the factor  $\frac{1}{2}$  in the Serber force.<sup>47</sup> The factor  $(2\pi)^{-12}$  goes with the four integrals over momentum space, and 64 represents the possible spin-charge states of the three initial nucleons  $k_i$ ,  $k_j$ , and  $k_k$ . The denominator  $4(2\pi)^{-3} \int d^3 k$  reduces the result to an energy per nucleon. The negative sign arises from the fact that there are three attractive interactions.

Now the matrix elements (12.6) decrease rapidly with increasing  $q$ . Therefore, if the  $z$  axis is chosen to be in the direction  $q$ , the most important contributions will come from initial momenta  $k_i$  and  $k_k$  which have a positive  $z$  component, and momenta  $k_j$  with a negative  $z$  component, and particularly from states which lie

<sup>46</sup> P. C. Martin and J. Goldstone have independently pointed out to me that there is still another possible type of 3-particle cluster term: After the first intermediate state (12.4) is reached, the nucleon  $k$  fills the void left by nucleon  $i$ , while nucleon  $j$  takes up the momentum balance. This gives the alternative second intermediate state

$$k''_i = k_i - q; \quad k''_j = k_j + k_k - k_i + q; \quad k''_k = k_k.$$

The contribution from this alternative is likely to be of the same order as that from (12.5). [The possibility of letting nucleon  $k$  fill the state  $k_i$  does not give anything new because in this case  $k''_i = k_i + q$ ,  $k''_k = k_k$ , which is the same as state (12.5).]

<sup>47</sup> Brueckner has an additional factor  $\frac{1}{2}$  which presumably is meant to take into account that each pair  $ij$ ,  $jk$ , and  $ki$  in (12.3) is to be counted only once—as is well known, the sum over all pairs  $ij$  is equivalent to one-half the sum over  $i$  and  $j$  independently. However, in our case, the three states  $i$ ,  $j$ , and  $k$  are distinguishable by the order in which the nucleons get excited and de-excited. Thus  $i$  is the nucleon which gets excited in the first step but de-excited only in the last. Therefore we should let each of the three nucleons  $i$ ,  $j$  and  $k$  independently assume each of the possible  $A$  states.

close to the surface of the Fermi sphere—the latter assumption will also reduce the resonance denominators in (12.7). Thus the main contribution will come from rather restricted regions of the Fermi spheres for  $\mathbf{k}_i$ ,  $\mathbf{k}_j$ , and  $\mathbf{k}_k$ , and this is the main reason why the contribution  $\Delta E_3$  will turn out to be small.

If we assume that only these restricted regions of the Fermi sphere contribute appreciably, two simplifications are possible. First, the exchange terms  $f(\mathbf{k}_i - \mathbf{k}_j + \mathbf{q})$  and  $f(\mathbf{k}_k - \mathbf{k}_i + \mathbf{q})$  can be neglected because the momentum change in each case is about  $2k_F$ , and  $f(2k_F)$  is only about 0.1 [see Eq. (10.14)]. However, the last exchange term,  $f(\mathbf{k}_k - \mathbf{k}_j)$ , may be large. Secondly, the denominator may be approximated by

$$(\mathbf{k}_i - \mathbf{q})^2 + (\mathbf{k}_j + \mathbf{q})^2 - k_i^2 - k_j^2 \approx 2qk_F(\mu_i + \mu_j), \quad (12.8)$$

where  $\mu_i = \cos\theta_i$  [ $\theta_i$  being the angle between  $\mathbf{k}_i$  and the positive  $z$  axis ( $\mathbf{q}$  direction)], and  $\mu_j = \cos\theta_j$  ( $\theta_j$  being the angle between  $\mathbf{k}_j$  and the negative  $z$  axis). According to the argument of the last paragraph, both  $\mu_i$  and  $\mu_j$  are between 0 and 1. We have assumed in (12.8) that  $k_i$ ,  $k_j$ , and  $k_k$  are all close to  $k_F$ . In (12.8), a term quadratic in  $q$  is neglected; if it were included, the convergence of the integral for large  $q$  would become more rapid [see Eq. (12.20)]. With the same approximations,  $d^3k_i = 2\pi k_F^2 dx_i d\mu_i$ , where  $x_i = k_F - k_i$  may go from 0 to  $qu_i$ , again neglecting terms of order  $q^2$ , a neglect which again overestimates the integral. Putting also  $d^3q = 4\pi q^2 dq$ , we get then

$$\begin{aligned} \frac{\Delta E_3}{A} &= -\frac{16}{(2\pi)^3} \frac{M^{*2}}{M^3} (1.68a)^3 \frac{k_F^4}{\frac{1}{3}k_F^3} \int_0^\infty \frac{q^2 dq}{q^2} f^2(q) \\ &\times \int \int \int d\mu_i d\mu_j d\mu_k \int \int \int dx_i dx_j dx_k \\ &\times \frac{1}{\mu_i + \mu_j} \frac{1}{\mu_i + \mu_k} [f(q) + f(k_F(\mu_i - \mu_k))]. \end{aligned} \quad (12.9)$$

The integrations over  $x_i$ ,  $x_j$ , and  $x_k$  may be carried out, and  $f$  inserted from (12.6):

$$\begin{aligned} \frac{\Delta E_3}{A} &= -\frac{6}{\pi^3} \left(\frac{M^*}{M}\right)^2 (1.68a)^3 \frac{k_F}{M} \int_0^\infty \frac{q^3 dq}{(1+q^2a^2)^2} \\ &\times \int \int \int \frac{\mu_i d\mu_i \mu_j d\mu_j \mu_k d\mu_k}{(\mu_i + \mu_j)(\mu_i + \mu_k)} \\ &\times \left[ \frac{1}{1+q^2a^2} + \frac{1}{1+\alpha^2(\mu_i - \mu_k)^2} \right], \end{aligned} \quad (12.10)$$

with  $\alpha$  given by (10.14).

Brueckner has considered only the first term in the square brackets. The second term is somewhat more difficult to integrate; in fact, if (12.10) is taken literally,

the integral over  $q$  diverges for this term. But it is clear from the discussion above that the integrand has been greatly overestimated for  $q > k_F$ ; therefore it is reasonable to cut off the integral at about  $k_F$ , and in this case the contributions of the two terms in the square bracket will be about the same. Since only an estimate is wanted at present, we have considered only the first term in the bracket, integrating up to  $\infty$ , and have then doubled the final result.

The integrals over  $\mu_i$  and  $\mu_k$  are then elementary and alike, and the whole  $\mu$  integral becomes

$$\int_0^1 \mu_i d\mu_i \left[ 1 - \mu_i \ln \frac{1+\mu_i}{\mu_i} \right] = 0.089. \quad (12.11)$$

The  $\mu_j$  integral has here been evaluated numerically, which is probably the quickest way, and quite reliable since the integrand is almost constant at about 0.1 over the range from  $\mu_j = 0.2$  to 1. (Brueckner's result is 0.078.) The  $q$  integral gives  $1/4a^4$ , and

$$\frac{\Delta E_3}{A} = -2 \left(\frac{3}{2\pi^3}\right) \left(\frac{M^*}{M}\right)^2 (1.68)^3 0.089 \frac{k_F}{Ma}, \quad (12.12)$$

where the factor 2 has been inserted to take into account the second term in the bracket in (12.10).

This result is proportional to  $k_F$ , as is Brueckner's Eq. (73). Thus the three-particle clusters will not be very important for large  $k_F$  where the main part of the potential energy will be proportional to  $k_F^3$  if Serber forces are assumed; this is in agreement with our previous argument that these terms represent fluctuations in the effect of a third particle on the interaction of a pair and that the fluctuations become (relatively) smaller at higher density. For low density, on the other hand, although the *absolute* value of (12.12) decreases (in accord with the discussion in the beginning of this section), its *relative* importance becomes greater. This means that the independent-nucleon picture is then relatively more perturbed by the "cluster" term. As the density is lowered, a point will be reached where the cluster terms are so important that the approximation scheme of this paper no longer applies. It will then be a better starting point to assume that the nucleons associate in *actual* clusters, i.e., that we have a number of  $\alpha$  particles widely separated from each other. That this is so will also be indicated by the fact that the energy of a dilute nucleus, calculated according to the prescriptions of this paper, will turn out to be higher than that of an assembly of noninteracting  $\alpha$ -particles. Thus we see that the tendency to cluster formation at low density will be automatically indicated by the formalism. Conversely, the calculation at normal nuclear density indicates (see below) that the cluster terms are not important. This we consider as the best possible proof of the "shell-model" approximation used in this paper. We do not think it is necessary to make an additional *physical* assumption that clusters are

absent<sup>48</sup> at normal nuclear density, but we consider this a purely mathematical result of the theory.

With our adopted constants,  $k_F/Ma=45$  Mev, and (12.12) becomes

$$\Delta E_3/A = -1.8(M^*/M)^2 \text{ Mev.} \quad (12.13)$$

Tentatively, we may adopt for  $M^*/M$  the value obtained in Sec. XI, Table I, for the observed nuclear density, *viz.*, 0.6. Then

$$\Delta E_3/A = -0.66 \text{ Mev.} \quad (12.14)$$

This is approximately 100 times Brueckner's result, Eq. (74),

$$(\Delta E_3/A)_{\text{Brueckner}} = -0.007 \text{ Mev.} \quad (12.15)$$

Of this discrepancy, a factor of 8 is explained by the counting of states.<sup>47</sup> A factor of 2 disappears in Brueckner's calculation between his Eqs. (71) and (73). Another factor of 2 was introduced by us in (12.12) to take into account the second term in the bracket in (12.10). A factor of  $0.089/0.078 = 1.14$  comes from the evaluation of the angular integral (12.11). There is some difference in the choice of constants, which accounts for a factor 1.3 in the same direction. Finally, our evaluation of Brueckner's Eq. (73) with his constants gives 0.013 Mev.

Our result (12.14) is small but not spectacularly so. It will be greatly reduced if we take into account the previously deduced fact that actually only 12, rather than 64, spin-charge states contribute; then

$$\Delta E_3/A = -0.12 \text{ Mev,} \quad (12.16)$$

which gives about 1% correction to the binding energy. Since this is no longer entirely negligible, it would be desirable to repeat the calculation more accurately, especially the integration of (12.7). The actual result will be probably somewhat smaller than 0.12 Mev.

The result may be compared with the first-order average potential energy which is about 30 Mev at the actual nuclear density (Sec. XI, Table I), and with the second-order contribution which comes from the difference between  $G'$  and  $v'$  in (10.12) and which is 4% of the first order (with the assumed value  $M^*/M=0.6$ ) and hence about 1.2 Mev. Thus the third-order term, (12.16), falls rather well in line with the first two orders. This result is far more plausible than that implied in Brueckner's papers: in his calculation, the second order was about as large as the first because the Pauli principle had not been taken into account, while the third-order correction (12.15) was about 1 part in 4000 of the potential energy.

Our separation into first, second, third, . . . order is of course only valid for "well-behaved" potentials for which the  $G$  matrix can be expanded into a rapidly convergent series in powers of  $v$ , as shown in Sec. X. For potentials with repulsive cores this expansion is

impossible because the matrix elements of  $v$  do not exist while those of  $G$  do. The cluster expansion, on the other hand, remains meaningful. Brueckner *et al.* considered primarily potentials with repulsive cores; therefore the idea of comparing the cluster expansion with the expansion of  $G$  could not occur to them. However, it remains gratifying that for potentials for which  $G$  can be expanded, the various orders of this expansion and of the cluster expansion form a sequence which converges quite regularly.

We may then expect the next order, i.e., the four-particle cluster term, to be again about 10% of the third order. If we assume that there is no benefit from spin factors, i.e., nothing comparable to the factor 12/64 of the three-particle clusters, (an assumption which is quite unreasonable), the fourth order may be about 10% of (12.14) which would make it about half as large as the third order. The higher order terms would then be definitely smaller. The sign of each order is negative: In the  $n$ th order, (12.1) contains  $n$  interaction terms (negative), and  $n-1$  energy denominators (also negative). This result as well as the estimates of orders of magnitude should of course be checked by actual calculation.

Even though our result (12.16) for the three-particle cluster terms is not spectacularly small, it is still small enough to make the calculation without this correction very accurate. Moreover, this correction is merely a correction in the total binding energy and will probably not affect very much the relative positions of nuclear energy levels.

That  $\Delta E_3$  is so small is of course largely due to the Pauli principle, as already pointed out by Brueckner. The action of this principle greatly reduces the part of momentum space which can contribute appreciably. Only the halves of the Fermi spheres for which  $k_{js}$  and  $k_{ks}$  are positive, and  $k_{is}$  negative, will contribute, and the main contributions come from the neighborhood of the "poles" of the Fermi spheres, i.e.,  $k_{js}$ ,  $k_{ks}$ , and  $-k_{is}$  nearly equal to  $k_F$ . These geometrical restrictions make the integral (12.11) as small as 0.09. The restrictions, of course, exist only because the Fourier transform of the potential, (12.6), is quite small when the momentum of the nucleon changes from one side of the Fermi sphere to its opposite pole, i.e., when  $q=2k_F$ . The great effect of the Pauli principle therefore again depends on the relatively high density of the nucleus, compared to the relatively long range of nuclear forces.

We shall now consider some other forms of the interaction between particles. The first is the Coulomb force. In this case, the factors  $(1+q^2a^2)^{-1}$  in (12.10) will be replaced by  $q^{-2}$ . Then the integral will diverge for small  $q$ , a result which is clearly due to the long range of the Coulomb force. It might possibly be remedied by using the scattering matrix  $G'$  for the Coulomb field, rather than the potential matrix  $v'$ .

The second type of interaction is one which is more

<sup>48</sup> Contrary to R. J. Eden, reference 20, Sec. III.

important for nuclei, *viz.*, a repulsive core. In this case, the matrix  $I$  in (12.3) must not be replaced by the interaction matrix  $\nu$  but must be used directly. BG<sup>23</sup> show that the scattering matrix for two nucleons whose center of mass is at rest may be written

$$(k', -k' | G' | k, -k) = \int w_k(y) e^{-ik' \cdot r} d^3y, \quad (12.17)$$

where  $w$  does not depend strongly on  $k$ . If the radius of the repulsive core  $r_c$  is small so that  $k_p r_c < 1$  (which is well fulfilled for the actual dimensions), then

$$w_k(y) = \delta(y - r_c)/r_c, \quad (12.18)$$

where  $\delta$  is the ordinary, one-dimensional  $\delta$  function. Then  $G'$  is independent of  $k$ , and presumably also independent of the assumption that the center of mass is at rest, and we have with abbreviated notation

$$(k' | G' | k) = 4\pi \sin(k' r_c)/k'. \quad (12.19)$$

This takes the place of (10.8), and  $k'$  is nearly equal to  $q$ .

The main concern one might have in connection with a repulsive core is that the contribution from large  $q$  might diverge, or at least be very large. We therefore investigate (12.7), with the changed expression (12.19) for the matrix element, for large  $q$ . In this case, the previous approximation (12.8) for the energy denominator is not satisfactory but the energy denominators may instead be replaced by  $2q^2$  each. The integrals over  $k_i$ ,  $k_j$ , and  $k_k$  each give a factor  $(4\pi/3)k_F^3$ . The effective mass  $M^*$  for high  $q$  should be put equal to  $M$ . The term  $-2\pi \times 1.68a[f(q) + f(k_i - k_j + q)]$  and the corresponding term with  $k_k$ , will each be replaced by (12.19). Further,  $-2\pi \times 1.68a f(k_k - k_i)$  will be replaced by the limit of (12.19) for small  $k'$ , *viz.*,  $4\pi r_c$ , and  $f(q)$  may be neglected by comparison. Finally, we change the 64 in (12.7) to the more correct value 12, see above. Then (12.7) is replaced by

$$\frac{\Delta E_s}{A} = \frac{12}{M} \frac{(2\pi)^{-9}}{M} \left( \frac{4\pi}{3} k_F^3 \right)^2 (4\pi)^2 r_c 4\pi \times \int \frac{q^2 dq \sin^2(qr_c)}{4q^4 - q^2}. \quad (12.20)$$

This integral clearly converges at large  $q$  and the main contribution comes from near the lower limit. This limit we put arbitrarily equal to  $2k_F$ , which is about the point where our approximations become seriously wrong. Then, assuming  $k_F r_c \ll 1$ , we obtain

$$\frac{\Delta E_s}{A} = \frac{4}{3\pi^2} \frac{k_F^2}{M} (k_F r_c)^3. \quad (12.21)$$

Using  $r_c = 0.6 \times 10^{-12}$  cm, and our old value  $k_F = 1.29 \times 10^{12}$  cm<sup>-1</sup>, this gives 1.37 Mev. However, for these values of the constants,  $k_F r_c$  is actually not very small, and more accurate evaluation gives a correction factor

of about 1/3, or  $\Delta E_s/A = 0.45$  Mev. This is larger than the result (12.16) for the attractive Yukawa potential but still a rather small correction, leaving the Brueckner theory a very good approximation.

It will be noted that (12.21), arising from a repulsive interaction, is positive while (12.16), coming from an attractive interaction, is negative. There will thus be partial compensation of these contributions, as was pointed out by Brueckner.<sup>49</sup> Further calculations will be necessary to establish the actual correction terms from 3-particle and larger clusters; for the time being, the best estimate is a few hundred kev, and the sign is uncertain.

### XIII. THE DEPENDENCE ON THE MASS NUMBER $A$

Brueckner<sup>15</sup> has shown that the leading term in the energy of a large nucleus is proportional to its mass number  $A$ . This result—which is correct under his assumptions—has given rise to considerable discussion because it is well known that the energy of certain systems is not proportional to the number of particles; e.g. the energy of an atom with  $Z$  electrons is proportional to  $Z^{7/3}$ . Only if the forces in the system saturate should the actual binding energy be proportional to  $A$ .

The point is that Brueckner tacitly assumes that the density of particles is held constant as the size of the system is increased. With this assumption, the result  $E \sim A$  is most plausible, in fact nearly obvious.<sup>50</sup> Now as we have discussed in Sec. IX, calculating the energy at given density gives merely a formal solution of the problem. To get the actual self-consistent solution, we must find the minimum of the energy as a function of density. Now if the forces saturate, then the density tends to a definite limit for large number of particles, and then the actual binding energy will also be proportional to  $A$ . This corresponds to the observed behavior of nuclei. If, however, the forces do not saturate, the density itself will increase with  $A$ , and the binding energy per particle will do likewise.

A convenient example of a nonsaturating force is the gravitational interaction, i.e., an attractive potential  $-g^2/r$  between any two particles. The self-consistent problem for this case is easy to formulate, and not very difficult to solve. If the number of particles is very large, the Fermi statistical method may be used, and the problem then becomes similar to the Fermi-Thomas statistical distribution of the electrons in an atom. There are two differences, however: (a) the interaction between the particles is attractive rather than repulsive, and (b) there is no central body attracting the particles.

<sup>49</sup> Private communication through R. J. Eden.

<sup>50</sup> Nevertheless, this result represented great progress. The Brillouin-Wigner perturbation theory expansion, in which the energy denominators are  $E - H_0$ , with  $E$  the exact eigenvalue and  $H_0$  the unperturbed Hamiltonian, gives in fourth-order terms proportional to  $A^4$ , in the sixth-order proportional to  $A^6$ , etc. [K. A. Brueckner (private communication) and BC]. In BC it was shown for the first time that these divergences with  $A$ , which must be spurious on physical grounds, do in fact cancel if  $E$  is replaced by the unperturbed energy.

Exactly the same problem as ours occurs in the theory of the density distribution in a white dwarf star<sup>a</sup> in which we have a degenerate electron gas held together by gravitational forces.<sup>b</sup>

If relativistic effects are neglected, we can easily calculate the radius  $R$  of the sphere containing  $A$  particles interacting by gravitation. The kinetic energy per particle is proportional to  $k_F^2$ , where  $k_F$  is the Fermi momentum. The potential energy per particle is the gravitational potential which is proportional to  $A/R$ , where  $R$  is the radius of the sphere. The density is  $\rho \sim A/R^3$  and  $k_F^3$  is therefore proportional to  $A/R^3$ ; hence the potential energy is proportional to  $A^{2/3}k_F^3$  and the total energy proportional to

$$\mathcal{E} = \frac{1}{2}k_F^2 - cA^{2/3}k_F, \quad (13.1)$$

where  $c$  is a constant. The minimum of this expression is obtained for

$$k_F = cA^{2/3}. \quad (13.2)$$

The other quantities then depend on  $A$  as follows:

$$R \sim A^{1/3}/k_F \sim A^{-1/3}, \quad \rho \sim A^{-3} \sim A^2, \quad \mathcal{E} \sim A^{4/3}. \quad (13.3)$$

The volume of such a sphere is thus inversely, rather than directly, proportional to the number of particles. The radius behaves just as in the Fermi-Thomas atom where the mean radius is proportional to  $Z^{-1/3}$  and the total energy goes as  $A^{7/3}$ , which is also the same as in the Thomas-Fermi atom.

The behavior just described will also be obtained from the Brueckner method because it, just like the Hartree method, has the Fermi-Thomas model as its limit for high particle density. Thus the actual binding energy in our example is by no means proportional to  $A$ , but to a much higher power; but this does not necessarily affect Brueckner's proof that at given density, the energy is indeed proportional to  $A$ .

This last statement has to be qualified, however, by the condition that the energy per particle must be finite in an infinite system if the density is kept constant. This condition remains satisfied if the interaction does not saturate but has finite range. But for Coulomb forces, with their effectively infinite range, it is not satisfied: The gravitational potential at the center of a sphere of radius  $r$  at constant density is proportional to  $r^2$  and therefore does not tend to a finite limit as  $r$  increases.

#### XIV. TERMS OF ORDER 1/A

In Sec. III we stated that certain correction terms were of relative order 1/A, and hence negligible in comparison with the main term for large nuclei. We shall now discuss these terms. In this section, we shall consider only those matrix elements which conserve

<sup>a</sup> S. Chandrasekhar, Monthly Notices Roy. Astron. Soc. 95, 207 (1935).

<sup>b</sup> It does not matter that the gravitation acts primarily on the nuclei in the white dwarf because nuclei and electrons are closely tied together by the (much stronger) electric forces.

momentum, as is required for an infinite nucleus; those which do not conserve momentum will be discussed in the next section. We shall first discuss the diagonal elements of the correction terms for the chosen configuration, and then, very briefly, the nondiagonal terms which mix the model states.

We shall here consider the terms  $w_2$  and  $w_3$ , Eqs. (4.15) and (4.16). These terms were already considered by BL, Sec. III. We shall follow their argument, but with the important difference that we consider the matrix element

$$(\Phi_C, w_m \Phi_C), \quad (14.1)$$

while they used

$$(\Psi_C, w_m \Phi_C). \quad (14.2)$$

It was shown in footnote 25 that the use of (14.2) is incorrect, and we shall show now that (14.1) is much simpler and gives a much smaller result than (14.2).

The diagonal element of  $w_2$  is

$$\begin{aligned} (\Phi_C, w_2 \Phi_C) &= - \sum_{ii} \left( \Phi_C, \tilde{G}_{ij} \frac{Q}{e} I_{ij} L_{ij} \Phi_C \right) \\ &= - \sum_{ii} \left( \frac{Q}{e} \tilde{G}_{ij} \Phi_C, I_{ij} L_{ij} \Phi_C \right). \end{aligned} \quad (14.3)$$

But  $\tilde{G}_{ij}$ , according to its definition, (7.4), (7.10), and (7.11), can excite at most one nucleon out of the chosen configuration. On the other hand,  $I_{ij}$  operating on  $\Phi_C$  must excite both nucleons. Therefore, at least if  $L_{ij}$  is replaced by 1, Eq. (14.3) gives exactly zero. The first nonvanishing contribution is of the three-particle cluster type, viz.:

$$\sum_{ijk} \left( \Phi_C, \tilde{G}_{ij} \frac{Q}{e_{ij}} I_{ij} \frac{Q}{e_{jk}} I_{jk} \frac{Q}{e_{ki}} I_{ki} \Phi_C \right), \quad (14.4)$$

where  $\tilde{G}_{ij}$  excites either nucleon  $i$  or  $j$  only. Of the  $I$  operators, at least one must violate momentum conservation;  $\tilde{G}$  does the same, and it is shown in Sec. XV that each such operator introduces at least a factor  $A^{-1}$ . Thus (14.4) will be at least a factor  $A$  smaller than the analogous term (14.7) below, and is therefore entirely negligible. In BL, on the other hand, this term gives the main contribution, Eq. (26), which they evaluate to be about 10 Mev for the whole nucleus (their Appendix B).

The diagonal element of  $w_3$  is

$$\begin{aligned} (\Phi_C, w_3 \Phi_C) &= - \sum_{ii} \left( \Phi_C, v_{ij} \frac{Q}{e_{ij}} \tilde{G}_{ij} L_{ij} \Phi_C \right) \\ &= - \sum_{ii} \left( \frac{Q}{e_{ij}} v_{ij} \tilde{G}_{ij} \Phi_C, L_{ij} \Phi_C \right). \end{aligned} \quad (14.5)$$

The operator  $v_{ij}$ , in contrast to  $\tilde{G}_{ij}$  in (14.3), can excite both nucleons  $i$  and  $j$ , and the operator  $\tilde{G}_{ij}$  will then leave the two nucleons excited. The structure of (14.5)

is therefore analogous to the cluster term (12.1) except that  $I_{ij}$  has been replaced by a more complicated expression,

$$-\tilde{G}_{ij} \frac{Q}{e_{ij}} v_{ij}. \quad (14.6)$$

The lowest order nonvanishing contribution to (14.5) is therefore, in analogy to (12.3), the three-particle cluster term

$$w_{33} = -\sum \left( \Phi_C, \frac{Q}{e_{ij}} \tilde{G}_{ij} \frac{Q}{e_{ik}} I_{jk} \frac{Q}{e_{ki}} I_{ki} \Phi_C \right). \quad (14.7)$$

Now (14.7), or the more general expression (14.5), can easily be combined with (12.3) or (12.1), respectively, if we replace  $v_{ij}$  by  $I_{ij}$ . As we have seen in Sec. X, the  $v$  matrix is not very different from the  $G$  matrix if the potential is well-behaved, and the elements of  $v_{ij}$  which lead to the excitation of two nucleons are essentially equal to the corresponding elements of the  $I$  matrix, Eq. (7.5). Writing then

$$L_{ij} - 1 = \frac{Q}{e_{ij}} L_{ij}' \quad (14.8)$$

[the term 1 in  $F_{ij}$  gives no contribution to either (12.1) or (14.5)], we get for the sum of (12.1) and (16.5):

$$\begin{aligned} & \left( \Phi_C, \sum_{ij} I_{ij} \left( \frac{Q}{e_{ij}} - \frac{Q}{e_{ij}} \tilde{G}_{ij} \frac{Q}{e_{ij}} \right) L_{ij}' \Phi_C \right) \\ & \approx \left( \Phi_C, \sum_{ij} I_{ij} \frac{Q}{e_{ij} + \tilde{G}_{ij}} L_{ij}' \Phi_C \right), \end{aligned} \quad (14.9)$$

where in the last line it has been assumed that  $\tilde{G}_{ij} \ll e_{ij}$ , as will be shown to be indeed the case. Thus the only effect of  $w_3$  is to modify the first denominator in the cluster terms by adding  $\tilde{G}_{ij}$ .

Now  $\tilde{G}_{ij}$  is essentially the same as the diagonal element of  $v_{ij}$ . This was calculated in (6.4) and found to be proportional to  $\Omega^{-1}$  or  $A^{-1}$ . This shows that the  $\tilde{G}_{ij}$  in (14.9) gives a correction of the order of  $1/A$ , since  $e_{ij}$  is independent of  $A$ . The term  $w_3$  is therefore of order  $1/A$  compared with the cluster terms, and using the estimates of Sec. XII for the latter, we see that  $w_3$  is of the order of a few hundred kev for the whole nucleus, which is clearly negligible.

The reason for the smallness of  $w_3$  is the occurrence of the operator  $\tilde{G}_{ij}$  in (14.5). This operator is of order  $\Omega^{-1}$ , which has to be compared with the denominator  $e_{ij}$  which occurs associated with it and which is independent of  $\Omega$ . It may be argued that the  $I_{ij}$  occurring in (12.1) are also of order  $\Omega^{-1}$ : But  $I_{ij}$ , being a non-diagonal element, leaves open the choice of the momentum change  $q$ , (see Sec. VI), and the number of choices of  $q$  is proportional to  $\Omega$ . On the other hand,  $\tilde{G}$  is a diagonal element and thus permits no choice of final state.

In spite of the smallness of  $w_3$ , it is interesting to investigate the meaning of the change of the denominator in (14.9). According to (7.3),

$$(n, n_j | \tilde{G}_{ij} | n, n_i) = (n, n_j | G_{ij} | n, n_i), \quad (14.10)$$

and this is the first term in  $\Delta G_{ij}$ , Eq. (3.6), which is a small correction to the excitation energy  $-e_{ij}$ , Eq. (3.4). Thus, according to (14.9), the interaction between the two excited nucleons  $ij$  should be omitted in the first (but not the other), resonance denominator  $e_{ij}$  when calculating the cluster term  $\Delta E_3$ . This takes into account all the small ( $1/A$ ) corrections of Sec. IV provided we put  $v = G$  in these corrections.

The nondiagonal terms,

$$(\Phi_B, w_m \Phi_C), \quad (14.11)$$

are important because they indicate to what extent the "improved" model wave function  $\Phi'$ , Eq. (4.6), differs from the simple model wave function  $\Phi_C$  defined in Sec. II. We have shown in Sec. IV and in EB that  $w_1$  has essentially no nondiagonal elements if the chosen configuration is nondegenerate. Therefore we have to consider only  $w_2$  and  $w_3$ .

It can be shown fairly easily that  $w_2$  and  $w_3$  cause an admixture of "foreign" configurations  $B$  in the improved model wave function  $\Phi'$  which is only of order  $1/A$ . The corresponding second-order perturbation of the energy is then also of order  $1/A$ ; a rough estimate yields

$$\Delta E_{2,3}^{(2)} = \frac{\sum |\Phi_B, (w_2 + w_3) \Phi_C|^2}{E_C - E_B} \approx -\frac{2 \text{ Mev}}{A}, \quad (14.12)$$

which is completely negligible.

## XV. TERMS NOT CONSERVING MOMENTUM

In all our quantitative calculations, e.g., in Secs. VI and IX-XIV, we have assumed that the matrix elements of  $v_{ij}$  and  $G_{ij}$  are different from zero only if momentum is conserved, as in (2.8). This is of course not strictly true for a finite nucleus. In this section we shall estimate the magnitude of the matrix elements which do not conserve momentum, particularly those in which only one nucleon changes its state.

For this investigation, it is convenient to replace  $G_{ij}$  by  $v_{ij}$  (Sec. X). Then the required matrix elements are

$$(n, n_j | v_{ij} | n, n_i)_P$$

$$= \int d\tau_i d\tau_j \psi^*(n_i, \mathbf{r}_i) \psi^*(n'_j, \mathbf{r}_j) v_{ij}(\mathbf{r}_i - \mathbf{r}_j) \times \psi(n_i, \mathbf{r}_i) \psi(n_j, \mathbf{r}_j). \quad (15.1)$$

It is convenient to define a quasi-potential acting on particle  $j$ , thus:

$$u_{ij}(\mathbf{r}_j) = \int d\tau_i |\psi(n_i, \mathbf{r}_i)|^2 v_{ij}(\mathbf{r}_i - \mathbf{r}_j). \quad (15.2)$$

In a nucleus of volume  $\Omega$ ,  $|\psi|^2$  is of order  $\Omega^{-1}$  and  $u(r_i)$  for any given point  $r_i$  will be of the same order, due to the assumed finite range of  $v_{ij}$ . The diagonal element of  $v_{ij}$ ,

$$\langle n_i n_j | v_{ij} | n_i n_j \rangle = \int d\tau_i u(r_i) |\psi(n_i, r_i)|^2, \quad (15.3)$$

will then be of the same order  $\Omega^{-1}$  since  $|\psi|^2$  is of order  $\Omega^{-1}$  and the whole nuclear volume  $\Omega$  gives a positive contribution.

To estimate the nondiagonal terms, we use closure, thus:

$$\begin{aligned} \sum_{n'_j} |(n_i n_j' | v_{ij} | n_i n_j)|^2 \\ = \sum_{n'_j} \left| \int d\tau_j \psi^*(n_j', r_j) u(r_i) \psi(n_j, r_j) \right|^2 \\ = \int d\tau_j |u(r_j)|^2 |\psi(n_j, r_j)|^2. \end{aligned} \quad (15.4)$$

Since  $u$  and  $|\psi|^2$  are each of order  $\Omega^{-1}$ , the integrand is  $\Omega^{-3}$  and the integral over the nuclear volume is  $\Omega^{-2}$ . Thus the sum in (15.4) is of the same order of magnitude as the single term  $n_j' = n_j$ , which is the square of (15.3). In other words, all the nondiagonal terms together contribute about as much to (15.4) as the single diagonal term.

The number of nondiagonal terms  $n'_j$ , however, is proportional to  $\Omega$  since  $\sum_{n'_j}$  may be replaced by  $(2\pi)^{-3} \int d^3 k / k^3$ . Hence each individual term  $n'_j$  gives a contribution of order  $\Omega^{-3}$  to (15.4), or the matrix element (15.1) is of order  $\Omega^{-3/2}$ . This compares with  $\Omega^{-1}$  for the matrix elements which conserve momentum (Sec. VI), and thus shows that indeed the elements in which only a single nucleon is excited, become small for large nuclei. The same is true for matrix elements in which both nucleons are excited but momentum is not conserved.

If we calculate, for example, the contribution to the cluster term  $\Delta E_3$  which comes from matrix elements which do not conserve momentum, then at least two such elements must be involved, and the resulting contribution is at least by a factor  $A$  smaller than that calculated in Sec. XII.

An even closer estimate than (15.4) may be made for the nondiagonal matrix elements of the one-nucleon potential  $V$ . With our assumption  $G_{ij} = v_{ij}$ , and with the definition (15.2), we have

$$\begin{aligned} V(r_i) &= \sum_i u_{ij}(r_i) = \int d\tau v(r - r_i) \sum_i |\psi(n_i, r)|^2 \\ &= \int d\tau \rho(r) v(r - r_i), \end{aligned} \quad (15.5)$$

where  $\rho$  is the total density of nucleons. Now for a

large nucleus,  $\rho$  is very nearly constant ( $= \rho_0$ ) over the interior of the nucleus. Only in a surface layer of relative volume of order  $A^{-1/3}$ , does  $\rho$  become appreciably smaller than  $\rho_0$ . To estimate the nondiagonal elements (7.9) of  $V$ , we therefore form, similarly to (15.4):

$$\begin{aligned} \sum_{n'_j \neq n_j} |(n_j' | V | n_j)|^2 \\ = \int d\tau [V(r_j)]^2 |\psi(n_j, r_j)|^2 - \langle V \rangle^2 \\ = \int d\tau [V(r_j) - \langle V \rangle]^2 |\psi(n_j, r_j)|^2, \end{aligned} \quad (15.6)$$

where

$$\langle V \rangle = \int V(r_j) |\psi(n_j, r_j)|^2 d\tau_j \quad (15.7)$$

is the expectation value of the potential. Now in the interior,  $V(r_j) - \langle V \rangle$  is of order  $A^{-1/3}$  so that the contribution of the interior to (15.6) is of order  $A^{-2/3}$ . The main contribution comes from the surface layer and is proportional to the relative volume of that layer,  $A^{-1/3}$ .

Thus the sum is (15.6) is of order  $A^{-1/3}$ , and is smaller by this factor than the diagonal term  $(n_j | V | n_j)^2$ . Since the number of terms is again proportional to  $A$ , an individual term  $(n_j' | V | n_j)$  will only be of order  $A^{-2/3}$  compared with the diagonal term.

#### XVI. PROBLEMS FOR A FINITE NUCLEUS

In Secs. II, III, and VII we have developed the general method for a finite just as for an infinite nucleus. In Secs. XIV and XV we have shown that the correction terms which may arise for a finite nucleus, are small. Nevertheless, many further problems will have to be solved before reliable quantitative results can be obtained.

The first step in treating a finite nucleus is the choice of a potential to start the self-consistent calculation of Sec. II. This is far more difficult than in the Hartree method for two reasons: First, the whole potential concept is somewhat invalidated by the complications discussed in Sec. III, but we have shown at the end of Sec. X that these complications are not very important quantitatively, at least for "well-behaved" interactions. Second, we have to know a potential matrix  $(r' | V | r)$ , rather than a simple potential  $V(r)$ .

To determine the potential matrix in a finite nucleus combines the problems of finding the Hartree potential for an atom and the Brueckner potential for an infinite nucleus. The Hartree potential is diagonal in position,  $V(r)$ , and when transformed to momentum space, depends only on the difference  $|k' - k|$ . The Brueckner potential for an infinite nucleus (Secs. IX to XI) is a function of momentum only,  $V(k)$ , and if transformed to coordinate space, will depend only on the distance  $|r' - r|$ ; these two are therefore complementary. The potential matrix in a finite nucleus will be neither

diagonal in position nor in momentum, and will thus depend on  $r' - r$  as well as  $r' + r$ , and on  $k' + k$  as well as  $k' - k$ .

There remains, however, a simplifying feature which will probably be very important for the actual solution. The dependence on  $r' + r$  is designed to simulate the conventional potential well; the potential  $V$  will therefore drop when  $\frac{1}{2}|r' + r|$  exceeds the nuclear radius  $R \approx r_0 A^{1/3}$ . On the other hand, the dependence on  $r' - r$  is to represent the momentum-dependence of the Brueckner potential  $V(k)$  for an infinite nucleus. Now  $V(k)$  changes appreciably when  $k$  goes from 0 to  $k_F$ ; therefore the Fourier transform  $V(r' - r)$  will change appreciably when  $|r' - r|$  goes from 0 to  $1/k_F$ , which is about  $r_0$ . For a large nucleus, therefore, much larger distances are involved in  $|r' + r|$  than in  $|r' - r|$ , and the two dependences can be separated (except in the region of the nuclear surface). For a small nucleus, the determination of  $(r'|V|r)$  is likely to be much more difficult.

The wave functions of the nucleons will be determined mainly by the large-scale behavior of  $V$ , i.e. by its dependence on  $r' + r$ . For a first approximation, therefore, one can probably take simply

$$(r'|V|r) = V(r)\delta(r' - r),$$

in other words an old-fashioned Hartree type potential, and determine the wave functions in this potential by solving (2.3). In other words, one may go back to the standard procedure in shell-model theory. Of course, once the wave functions of the nucleons have been determined, one must then find the reaction matrix using (3.1) and one will thus obtain a velocity-dependent potential, just as for an infinite nucleus. This potential will *not* agree with the Hartree potential used at the start, but when wave functions are calculated in this new potential, it is hoped that they will not differ too much from those calculated in the first approximation.

The accurate determination of the potential matrix  $(r'|V|r)$  in the region of the nuclear boundary is obviously a very difficult problem. To solve it, it will probably be best to consider first the problem of an infinite plane nuclear boundary and to solve the self-consistent problem for this. Then if the normal to the boundary is in the  $x$  direction, we may write

$$(r_1|V|r_1) = V(\frac{1}{2}(x_1 + x_2), x_1 - x_2, r_{12}). \quad (16.1)$$

It has been suggested by Skyrme<sup>58</sup> that one might consider the dependence on  $r_{12}$  to be similar to that for an infinite nucleus whose density is the same as that found at  $\frac{1}{2}(x_1 + x_2)$ . Solution of this problem of the nuclear boundary layer will yield the surface energy of the nucleus.<sup>59</sup>

Once the problem of the plane nuclear boundary is solved, the potential matrix for a finite nucleus may be

assumed to depend on the position coordinates  $r$ ,  $r'$  in the boundary layer in the same manner, i.e., it should be a good approximation to neglect the curvature of the nuclear surface. From the potential, one may then obtain the wave functions solving the Schrödinger equation (2.3).

Let us now assume that the wave functions of the individual nucleons have been determined. For the moment, we shall assume that the potential  $(r'|V|r)$  is spherically symmetric, i.e., that it depends only on  $r$ ,  $r'$ , and the angle between them (more about this later). Then the wave equation (2.3) separates in polar coordinates, and the nuclear wave functions  $\psi(n_i, r_i)$  should be the well-known shell model wave functions. In order to obtain the observed dependence on  $j$ , it must be assumed that  $V$  contains a term coupling spin and orbit, and it will be one of the tasks of the theory to derive such a term from the observed interaction between two nucleons.

If the chosen configuration  $C$  contains only closed shells, and corresponds to the ground state, the further calculation is essentially the same as for an infinite nucleus. It should be mentioned again, however, that configuration interaction is already contained in the method (reaction matrix); therefore the state of a closed-shell nucleus must *not* be considered as a mixture of various configurations, in an endeavor to lower its eigenvalue. The model wave function corresponds to one configuration  $C$  only.

Essentially the same statements hold for a nucleus containing one nucleon outside closed shells, or one less than a closed shell. This is analogous to the problem of an alkali atom.

If there are two or more nucleons in an incomplete shell, the situation is more complicated, just as in the corresponding case in the theory of atomic spectra. There are then many configurations of the nucleus which have the same energy, at least as long as we only consider the sum of the eigenvalues  $E(n_i^0)$  of the individual nucleons and disregard the interaction of the nucleons outside closed shells with each other. We therefore have to consider degenerate configurations; in fact the degeneracy is much higher than in the atomic case.

The most important consequence of degeneracy is that  $w_1$ , Eq. (4.14), now has many more nonvanishing matrix elements than in the absence of degeneracy, and that these appear in a much lower order of approximation. The operator  $1 - Q$  in (4.14) has the value unity for *all* configurations which are degenerate with the chosen configuration. We may thus consider the matrix element of (4.14) between the chosen configuration  $C$  and any other configuration  $B$  which is degenerate with it, *viz.*

$$(\Phi_B, w_1 \Phi_C) = \sum_{i,j} (\Phi_B, I_{ij} L_{ij} \Phi_C). \quad (16.2)$$

Now in contrast to the diagonal element (12.1) of  $w_1$ , the nondiagonal element (16.2) will in general not

<sup>58</sup> T. H. R. Skyrme (to be published).

vanish even if we set  $L_{ij}=1$ , its first approximation according to its definition (12.2). Then, in first approximation,

$$\langle \Phi_B, w_i \Phi_C \rangle = \sum_{ij} (\Phi_B, I_{ij} \Phi_C). \quad (16.3)$$

This is nonzero if  $B$  and  $C$  differ in the quantum states of two nucleons, which is indeed the most common case for two degenerate configurations. Assume, for example, that there are exactly two nucleons outside a closed shell of 50 nucleons; then these two nucleons may be in the  $3s$ ,  $2d$ , or  $1g_{7/2}$  shell. A state of total angular momentum 0 ( $S$  state) may be obtained from the configurations  $3s^2$ ,  $2d^2$ , or  $1g^2$ . To go from the first to the second of these configurations, the two nucleons ( $i$  and  $j$ ) have to be moved from an  $s$  to a  $d$  state which corresponds exactly to the matrix element (16.3). If there are more than two nucleons outside closed shells, we do not need to invoke the degeneracy of nucleon states of different  $l$ , such as the  $3s$ ,  $2d$ , and  $1g$  above, but even if all nucleons are within the same shell  $nl$ , there are many different configurations leading to the same total orbital momentum and spin,  $L$  and  $S$ , of the whole nucleus, which "interact" through matrix elements of the type (16.3).

Expression (16.3) is entirely analogous to the expression for the interaction of degenerate configurations in conventional shell-model theory. The only difference is that in the conventional theory  $I_{ij}=G_{ij}$  is replaced by  $v_{ij}$ , and according to Sec. X this does not make much difference for well-behaved potentials. For potentials with a repulsive core, it does make a difference, and in fact only the "modern" expression (16.3) is meaningful while the old-fashioned one with  $v_{ij}$  would not be. But the details of  $I_{ij}$  or  $v_{ij}$  do not actually matter; we are interested only in the matrix element (16.3) which depends on some over-all behavior of  $I_{ij}$ . This  $I_{ij}$  may well be replaced by an equivalent well-behaved potential which has the same matrix elements.

This is the more so since the most important matrix elements of (16.3),

$$\langle n'_i n'_j | G_{ij} | n_i n_j \rangle, \quad (16.4)$$

are those in which the states of the nucleons  $i$  and  $j$  (initial as well as final) are not very different. Then the product of the four wave functions involved in (16.4) will not change very rapidly with the distance  $r_{ij}$ , and the exact dependence of  $G_{ij}$  on  $r_{ij}$  will not matter much.

Thus our theory fully justifies<sup>54</sup> the conventional procedure of shell-model theory: the interaction between degenerate configurations is given by a very similar expression, and considerable freedom is allowed in the choice of the quasipotential  $v_{ij}$  which is to replace  $I_{ij}$ . Of course, it will be desirable in future shell-model calculations to choose  $v_{ij}$  so as to be compatible with

<sup>54</sup> When calculating operators other than the energy, it is of course necessary to take into account that the actual nuclear wave function differs from the model wave function, as has been described in Sec. VI.

the  $G_{ij}$  which has to be used in the Brueckner theory for an infinite nucleus, and which is derived from the interaction between two free nucleons in the manner described in Sec. X.

While the interaction between degenerate configurations thus reduces essentially to the conventional shell-model expression, the interaction between nondegenerate configurations is treated completely differently. In the conventional shell model, the matrix elements of the interaction corresponding to transitions from  $C$  to *any* other configuration would have to be calculated, and the resulting Hamiltonian matrix reduced to diagonal form, an essentially impossible task.<sup>55</sup> In our theory, all this part of the work is done in the first part of the procedure, i.e., when the scattering matrix  $G_{ij}$  for the two-nucleon system is determined by solving (3.1). After this is done, the configurations  $B$  which are not degenerate with  $C$  need no longer—in fact *must* no longer—be considered when the problem of the whole nucleus is set up. Thus the Hamiltonian matrix which has to be diagonalized for the nucleus is finite rather than infinite, and contains only the degenerate states. (Obviously, only states of the same total angular momentum  $J$ , and the same  $J_s=M$ , need to be considered.) Thus Brueckner's method separates the essentially insoluble problem into two simpler ones, that of determining the  $G$  matrix and that of reducing the Hamiltonian matrix for degenerate states only.

When solving (3.1) for a finite nucleus, the wave functions  $\psi(n, r)$  are of course shell-model wave functions, i.e., radial functions times spherical harmonics, not plane waves. However, because of the Pauli principle, the sum over  $n_i''$  and  $n_j''$  in (3.1) contains only unoccupied states which may be expected to be states of high momentum and to be not very different for a finite and for an infinite nucleus. Stated somewhat differently, the sum in (3.1) makes  $G_{ij}$  different from  $v_{ij}$  at small distances  $r_{ij}$ , of order  $r_0$  or less, and at these distances the over-all behavior of the wave functions, i.e., whether they are plane waves or spherical shell-model wave functions, should not matter very much. Thus it is to be hoped that the results from infinite nuclei can be taken over with little change.

We have made an essential distinction between degenerate and nondegenerate configurations. The question arises how to distinguish these in practice, especially because nucleon states like the  $3s$ ,  $2d$ , and  $1g_{7/2}$  mentioned above are almost but not exactly degenerate. Fortunately, there is great latitude in the definition of the operator  $Q$  in Sec. III, and this makes it a matter of our choice which of the configurations we wish to consider degenerate, and which not. For those in the former category, we set  $Q=0$ , which means that they are not taken into account as possible intermediate

<sup>55</sup> In practice, only a few other configurations are considered. This practice, adopted only for the sake of simplicity, is justified by our method.

states in calculating the scattering matrix  $G$  from (3.1); they will then give nonvanishing matrix elements (16.3) and thus have to be taken into account in the final Hamiltonian matrix of the complete nucleus. For the configurations which we wish to consider as nondegenerate with the former class, we set  $Q=1$ ; then they will contribute as intermediate states to the scattering matrix  $G$  in (3.1) but will not contribute elements (16.3) to the final Hamiltonian matrix.

It will presumably be convenient to include all configurations arising from particles in the same shell (in the sense of the shell model) as degenerate, and all others as nondegenerate. Thus if we have  $n$  particles outside the 50-shell, we distribute these in all possible ways over the 20 available places in the shells  $3s$ ,  $2d$ , and  $1g_{7/2}$  (and possibly also  $h_{11/2}$ ?), and consider all configurations arising in this way as degenerate. If one particle is put into the next higher shell, or a particle removed from the 50-shell and put into the  $sdg$  shell, the resulting configuration is considered as not degenerate with the former class, and assigned the value  $Q=1$ . Then the smallest denominators occurring in (3.1) will be equal to the energy difference between two successive shells. From the estimates in Sec. X it is likely that the contribution to  $G$  from configurations which have the smallest possible denominator will not be very large, and this fact justifies their inclusion among the "nondegenerate" configurations.

In contrast to the case of an infinite nucleus, the one-nucleon levels in a finite nucleus are discrete and the number of distinct shells is rather small. If we consider the nucleon shells  $n=1, 2, 3, \dots$  as closed at  $2, 8, 20, 28, 50, 82, 126, \dots$  nucleons, then from  $n=4$  up the total number of nucleons up to shell  $n$  is given by

$$N(n) = \frac{1}{2}n(n^2+5), \quad (16.5)$$

and the number of shells for a given mass number is roughly

$$n = (3A/2)^{1/3} \sim A^{1/3}. \quad (16.6)$$

The energy spacing between successive shells therefore decreases with  $A$  only as  $A^{-1/3}$ , and it is this slow decrease which makes the shell model so useful. The number of nucleons per shell goes up as  $A^{2/3}$ .

Furthermore, the matrix elements of  $v_{ij}$  or  $G_{ij}$  vary greatly from one nucleon pair to another. Two nucleons which have the same spatial wave function (and differ in spin or charge) will have a very large interaction, decreasing with atomic weight more slowly than  $1/A$ . Two nucleons in different shells, on the other hand, will have a considerably smaller interaction. Our estimates in Secs. VI and XV of the size of nuclear matrix elements must therefore not be taken seriously for individual matrix elements but hold only on the average.

The interaction between a pair of nucleons in the same shell depends greatly on the symmetry of the wave function with respect to the two nucleons. This

establishes a connection with the theory of multiplets developed by Wigner.<sup>56</sup> The only difference is that in our theory the multiplet structure, caused by the symmetry of the wave function, is subordinate to the shell structure for the individual nucleons, just as it is in atomic spectroscopy. This is of course quite familiar from the conventional treatments of the shell model. It is quite possible that the shell model with symmetry effects considered in second approximation, becomes a better approximation as the size of the nucleus increases, and that for very small nuclei (up to carbon, say) the original Wigner procedure, of considering symmetry first, is preferable.

The interaction between nucleons can presumably separate levels of the nucleus with different numbers of spatially symmetric pairs<sup>56</sup> very greatly, probably by more than the energy difference between successive nucleon shells. It may therefore be desirable to redefine the concept of "degenerate configurations" to take this symmetry effect at least partially into account. This will be important only when there are many nucleons in an incomplete shell.

If there are many nucleons in an incomplete shell, the "collective model" of Bohr and Mottelson<sup>57</sup> may become applicable. In our theory this means that a self-consistent solution will not be obtained for a spherically symmetric potential ( $r|V|r$ ) but for one of ellipsoidal shape. Since the self-consistent method is equivalent to a variational principle,<sup>58</sup> we may also say that the ellipsoidal shape gives a lower energy to the nucleus. Clearly this will happen only for certain distributions of the nucleons over the possible  $m$  values (magnetic quantum number) in the incomplete shell.

We have frequently stated that our method is applicable not only to the ground state but also to other states of the nucleus. For instance, all the configurations which are considered "degenerate" in first approximation, will be calculated simultaneously by diagonalization of the Hamiltonian matrix of the nucleus, as is customary in conventional shell-model theory. But also states in which one or more nucleons are excited to higher shells can be calculated. In this case, some of the denominators in the fundamental equation (3.1) will be negative because the intermediate state can have lower energy than the now chosen configuration. But this makes no difference: the main point is that states degenerate with the chosen one are always excluded by the operator  $Q$  so that no vanishing denominators can occur. Of course, the higher the excitation, the higher the degeneracy, so that it soon becomes impossible in practice to diagonalize the Hamiltonian. But at least a reliable method is provided for calculating statistical properties, such as the spread in energy of all the levels which arise for instance from a given

<sup>56</sup> E. P. Wigner, Phys. Rev. 51, 106 (1937). For a simple exposition, see J. M. Blatt and V. F. Weisskopf, *Theoretical Nuclear Physics* (John Wiley and Sons, Inc., New York, 1952), Chap. VI.

<sup>57</sup> A. Bohr and B. R. Mottelson, Physica 18, 1066–1078 (1952).

excitation of one nucleon, and perhaps also the distribution of these levels in energy. This will give a better basis for calculations of level density, and it may also be relevant to the giant resonance in the photoeffect.<sup>58</sup>

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#### APPENDIX. SPIN CONSIDERATIONS FOR THREE-PARTICLE CLUSTER TERMS

In this appendix, we shall consider the possible values of the spins of the three nucleons which interact according to Sec. XII. We shall consider wave functions which describe both spin and charge of a nucleon, and denote them by  $\alpha, \beta, \gamma$  for the three nucleons in the cluster. The orbitals of the three nucleons will be denoted by  $a, b, c$ . Then  $(aa, b\beta, c\gamma)$  denotes a possible assignment of spin-charge to the three orbitals;  $(a\beta, b\gamma, ca)$  would be another. The part of the wave function referring to the three nucleons (denoted 1, 2, 3) is the Slater subdeterminant

$$\psi_0 = (aa, b\beta, c\gamma) = \begin{vmatrix} a(1)\alpha(1) & b\beta(1) & c\gamma(1) \\ a(2)\alpha(2) & b\beta(2) & c\gamma(2) \\ a(3)\alpha(3) & b\beta(3) & c\gamma(3) \end{vmatrix}. \quad (\text{A.1})$$

*First step.*—We operate on the wave function (A.1) with the Serber operator

$$v\psi_0 = \frac{1}{2}v_{ab}(1 + P_{ab}), \quad (\text{A.2})$$

which gives

$$v\psi_0 = \frac{1}{2}v_{ab}[(aa, b\beta, c\gamma) + (ba, a\beta, c\gamma)], \quad (\text{A.3})$$

and take the matrix element leading to the first intermediate state

$$\psi_1 = (a'\alpha', b'\beta', c\gamma). \quad (\text{A.4})$$

Clearly, particle  $c\gamma$  must remain in the same state. It is sufficient to take the symmetry into account in the initial state, so we write

$$\psi_1 = a'\alpha'(1)b'\beta'(2)c\gamma(3). \quad (\text{A.5})$$

<sup>58</sup>D. H. Wilkinson, *Proceedings of the Glasgow Conference on Nuclear Physics, 1954* (Pergamon Press, London, 1955), p. 161.

Further, it is sufficient to take the part of (A.3) which assigns the state  $c\gamma$  to particle 3, then we have

$$\begin{aligned} v\psi_0 &= \frac{1}{2}v_{ab}[a\alpha(1)b\beta(2) + b\alpha(1)a\beta(2) \\ &\quad - b\beta(1)a\alpha(2) - a\beta(1)b\alpha(2)]c\gamma(3) \\ &= \frac{1}{2}v_{ab}[a(1)b(2) + b(1)a(2)] \\ &\quad \times [\alpha(1)\beta(2) - \beta(1)\alpha(2)]c\gamma(3). \quad (\text{A.6}) \end{aligned}$$

Clearly, the interaction is zero if  $\alpha = \beta$  as also shown in Sec. VIII. The integral over the coordinates of the third particle gives unity, and there is at this point no restriction on the spin  $\gamma$ .

The matrix element  $(\psi_1, v\psi_0)$  for  $\alpha \neq \beta$  will give a non-vanishing result in two cases:

I. If  $\alpha' = \alpha, \beta' = \beta$ , the matrix element comes from the term  $a(1)\beta(2)$  in (A.6) and is

$$(\psi_1, v\psi_0) = \frac{1}{2}(a'b' | v | ab) + \frac{1}{2}(b'a' | v | ab). \quad (\text{A.7})$$

II. If  $\alpha' = \beta, \beta' = \alpha$ , the matrix element comes from  $-\beta(1)\alpha(2)$  in (A.6) and is equal to (A.7) with opposite sign.

*Second step.*—Next we let particles  $b$  and  $c$  interact, in accord with the form of the three-cluster operator (12.3). This operation must bring a particle back to state  $b\beta$ . Thus the second intermediate state is

$$\psi_2 = (a'\alpha', b\beta, c'\gamma'). \quad (\text{A.8})$$

Since  $b$  and  $c$  interact, their spins in state  $\psi_1$  must be different, according to (A.6). Hence we must have

$$\gamma \neq \beta'. \quad (\text{A.9})$$

However, it is permissible that  $\gamma = \alpha'$  since particle  $a$  does not interact at this stage. We discuss separately the two cases defined above.

I. If  $\beta' = \beta$ , then (A.9) shows that  $\gamma \neq \beta$ . Then we must also have  $\gamma' = \gamma$ , Eq. (A.8), and the matrix element is

$$\frac{1}{2}(bc' | v | b'c) + \frac{1}{2}(c'b' | v | b'c). \quad (\text{A.10})$$

II. The two interacting particles have the spins  $\beta' = \alpha$  and  $\gamma$  in the first intermediate state, so we must have  $\gamma \neq \alpha$ . In the second intermediate state, their spins are  $\beta$  and  $\gamma'$ . Since the interaction does not contain spin, the spins  $\gamma, \alpha$  must match the spins  $\beta, \gamma'$ . Since we know that  $\alpha \neq \beta$ , the only possibility is that  $\gamma = \beta$ ; hence we must have  $\gamma' = \alpha$  and the states of the three particles are

$$\psi_0 = (aa, b\beta, c\beta), \quad (\text{A.11})$$

$$\psi_1 = (a'\beta, b'\alpha, c\beta), \quad (\text{A.12})$$

$$\psi_2 = (a'\beta, b\beta, c'\alpha). \quad (\text{A.13})$$

Then in going from  $\psi_1$  to  $\psi_2$ , the spins of the last two particles get interchanged, as they did in the first step of Case II. Thus, according to (A.6), the matrix element for the second step is the negative of (A.10).

*Third step.*—We let particles  $c$  and  $a$  interact, thus getting back to the initial state  $\psi_0$ .

Case I. Since the configuration in the second intermediate states is  $(a'\alpha, b\beta, c'\gamma)$ , application of (A.6) shows that  $\gamma \neq \alpha$ . Thus in case I, all three spins must be different. The matrix element is

$$\frac{1}{2}(ac|v|a'c') + \frac{1}{2}(ac|v|c'a'). \quad (\text{A.14})$$

Case II. The second intermediate state is given by (A.13). The requirement for (A.6) to be nonvanishing is now  $\alpha \neq \beta$  which is fulfilled anyway. The spins  $\alpha$  and  $\beta$  are interchanged again, so there is again a negative sign.

*General argument.*—We consider a triplet of orbitals  $a, b, c$  whose order is determined by the order of excitation. We have then the following possible spin assignments:

1. All 3 spins may be different. There are  $4 \times 3 \times 2 = 24$  possible assignments of spins to orbitals in this class. We then obtain Case I, and the complete matrix

element in the cluster is the product of (A.7), (A.10), and (A.14). This has been used in Sec. XII.

2. Two spins are equal, the third different.

(a) Particle  $b$  and  $c$  have equal spins; there are  $4 \times 3 = 12$  different assignments in this class. Then we have the situation of case II, Eqs. (A.11)–(A.13). The matrix element is the same as in case I, except for three negative signs.

(b) Particle  $b$  has the different sign. In this case, the matrix element is zero as can be seen by letting  $ac$  interact first. (12 possible assignments.)

(c) Particle  $c$  has the different spin. Again matrix element zero as shown by (A.6). 12 possible assignments.

3. All three spins equal. 4 possible values of this spin. Matrix element zero.

The total result is therefore  $(24 - 12)$  times the product of (A.7), (A.10), and (A.14).

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**Effect of a Repulsive Core in the Theory  
of Complex Nuclei**  
(with J. Goldstone)

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The effect of a repulsive core of infinite height on the wave function is not trivial (as it is for two free particles), but it can be calculated exactly. This is important because such a repulsive core does occur in the theoretical representation of the experiments on the interaction of two nucleons.

Results of the calculations of many people on the theory are reported in “Theory of Nuclear Matter” by H. A. Bethe, *Annual Rev. of Nuclear Sci.* **21**, 93–244 (1971).

## Effect of a repulsive core in the theory of complex nuclei

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Using Brueckner's method for the treatment of complex nuclei, the effect of an infinite repulsive core in the interaction between nucleons is studied. The Pauli principle is taken into account from the beginning. A spatial wave function for two nucleons is defined, and an integro-differential equation for this function is derived. Owing to the Pauli principle, the wave function contains no outgoing spherical waves. A solution is given for the case when only a repulsive core potential acts. The effective-mass approximation is investigated for virtual states of very large momentum.

### 1. INTRODUCTION

Considerable progress has recently been made in the treatment of the nuclear many-body problem by Brueckner and his collaborators (Brueckner & Levinson 1955; Brueckner 1955*a* and other papers<sup>†</sup>) and by Bethe (1956; this will be quoted as B). The determination of the energy of the nucleus is, in the main, reduced to the solution of a scattering problem which appears in the form of an integral equation (cf. B, equation (9·10)). If the interaction between two nucleons is of the 'conventional' type, i.e. everywhere attractive and of moderate strength, this equation can be solved by iteration (B, § X) and the solution is close to the Born approximation. For such interactions quite satisfactory results could be obtained by applying ordinary perturbation theory up to second (or perhaps third) order, as was done by Swiatecki (1956).

The most important application of Brueckner's method, however, is to a potential with a strong, possibly infinite, repulsive core. That such potentials act between two nucleons is strongly indicated (*a*) by the experimental results on proton-proton scattering (Jastrow 1951; Goldfarb & Feldman 1952), (*b*) by meson theory of nuclear forces (Lévy 1952) and (*c*) by the saturation requirement for nuclear forces in complex nuclei. An infinite repulsive core can certainly not be treated by perturbation theory because this would give an energy  $+\infty$  for the nucleus. Brueckner's work was therefore directed primarily towards such potentials (e.g. Brueckner 1955*a*). Apart from the Brueckner method, the variational method has been successfully applied to this problem by Jastrow (1955), and it will be interesting in the future to compare the results of the two methods.

Brueckner's first calculation (1955*a*) did not take into account the exclusion principle (e.p.). The effect of the e.p. is known to be very large for conventional potentials (B, § X), and the e.p. should therefore also be taken into account for a repulsive-core potential. This has been done by Brueckner & Wada (1956) in an approximate way: they solve the problem first without the e.p., and then take the

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‡ For further references to Brueckner's papers, see Bethe (1956).

e.p. into account by a perturbation-variation method. They further assume that the energy  $E(k)$  of a particle in the nuclear potential is given by the effective-mass approximation,  $E(k) = k^2/2M^*$ , and determine the effective mass by fitting the energy at the bottom and top of the Fermi distribution. It is somewhat doubtful whether these points are good choices (cf. § 6 of this paper). With their assumptions, Brueckner & Wada find a remarkably small effect of the e.p. on the total binding energy of a nucleus. This is partly due to a compensation: if the effective mass  $M^*$  were held constant, the e.p. would reduce the binding energy. But the e.p. also has the effect of increasing  $M^*$ , since it raises the lowest nucleon energy level very much and lowers the level  $k = k_F$  (B, § X; Brueckner & Wada). Increasing  $M^*$  in turn increases the binding energy.

In this paper we develop some direct methods for dealing with the repulsive core potential. We do not give any quantitative results for a physically reasonable potential, but we shall merely give the results for a pure repulsive core as an illustration.

## 2. DERIVATION OF THE SCHRÖDINGER EQUATION

We consider two nucleons in an infinite nucleus, having initially the momenta  $P + k_0$  and  $P - k_0$ , and after collision the momenta  $P + k'$  and  $P - k'$ . Then  $2P$  is the momentum of the centre of mass; in most of our calculations we shall set  $P = 0$ . We use the reaction matrix  $G$  defined in B, equation (9.10), and write

$$(P + k, P - k | G | P + k_0, P - k_0) \equiv (k | G | k_0, P). \quad (2.1)$$

Then  $G$  satisfies the integral equation B, (9.10)

$$\begin{aligned} & (k | G | k_0, P) \\ &= (k | v | k_0) - (2\pi)^{-3} \int_{k_F}^{\infty} d^3 k' Q \frac{(k | v | k') (k' | G | k_0, P)}{E(P+k') + E(P-k') - E(P+k_0) - E(P-k_0)}. \end{aligned} \quad (2.2)$$

Here  $Q$  denotes the principal value,  $v$  is the interaction between two nucleons and  $E(k)$  the energy of a nucleon of momentum  $k$ . The lower limit of the integral means that

$$|P + k'| > k_F, \quad |P - k'| > k_F, \quad (2.3)$$

where  $k_F$  is the Fermi momentum (see B, § X). Thus, if  $P \neq 0$ , the excluded volume in (2.2) is not spherical.

In (2.2) the reasonable assumption has been made that  $v$  depends only on the relative momenta of the interacting particles, not on the centre of mass momentum  $P$ . In particular, if  $v$  is an ordinary local potential  $v(x)$ , then the matrix elements of  $v$  are simply the Fourier transform of  $v$  (cf. B, equation (9.5)),

$$(k | v | k_0) = w(k - k_0) = \int v(x) e^{-ik \cdot k_0} \cdot x d^3 x, \quad (2.4)$$

and depends only on the difference  $k - k_0$ . It is sometimes convenient (see Brueckner & Wada (1956); also, De Dominicis & Martin, private communication), however

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to use a non-local interaction  $(y | v | x)$ ; then  $(k | \tilde{v} | k_0)$  depends on  $k$  and  $k_0$  separately and

$$(y | v | x) = \int (k | \tilde{v} | k') e^{ik \cdot x - ik' \cdot y} d^3 k d^3 k'. \quad (2.5)$$

We shall assume in this paper that  $v$  contains a repulsive core, i.e.

$$v(x) = +\infty \quad \text{for } x < r_c. \quad (2.6)$$

For the core radius, we shall usually assume Jastrow's (1951) best value

$$r_c = 0.6 \times 10^{-13} \text{ cm.} \quad (2.7)$$

We shall frequently use the dimensionless product  $k_F r_c$  which, using B, equation (9.13), has the value

$$c \equiv k_F r_c = 0.77. \quad (2.8)$$

Because of the repulsive core, the matrix elements (2.4) will be infinite so that (2.2) cannot be solved directly. Therefore we shall transform the integral equation (2.2) to co-ordinate space where the repulsive core can be introduced easily.

For this purpose, we first introduce a wave function  $\psi$  which we define in momentum space by

$$\psi(k) = (2\pi)^3 \delta(k - k_0) - (k | \tilde{G} | k_0, P) \frac{Q}{e} \theta, \quad (2.9)$$

where  $e$  is an abbreviation for the denominator† in (2.2) and  $\theta$  is a projection operator on the outside of the Fermi sphere, i.e.  $\theta = 1$  if (2.3) is fulfilled and  $\theta = 0$  otherwise. Of course  $\psi$  depends on  $k_0$  and  $P$  as parameters. Because of the occurrence of  $\theta$ ,  $\psi$  contains 'scattered waves' only in so far as they are permitted by the Pauli principle. We take the Fourier transform of (2.9),

$$\begin{aligned} \psi(x) &= (2\pi)^{-3} \int \psi(k) e^{ik \cdot x} d^3 k \\ &= e^{ik_0 \cdot x} - (2\pi)^{-3} \int (k | \tilde{G} | k_0, P) \frac{Q}{e(k)} e^{ik \cdot x} \theta d^3 k. \end{aligned} \quad (2.10)$$

The denominator

$$e(k) = E(P + k) + E(P - k) - E(P + k_0) - E(P - k_0) \quad (2.11)$$

has no singularities since  $P + k$ ,  $P - k$  both lie outside, and  $P + k_0$ ,  $P - k_0$  both inside the Fermi sphere. Therefore the operator  $Q$  may be replaced by 1. More important, the wave function contains no real scattered waves at all but only a distortion near the scattering centre. Physically this means that the Pauli principle forbids the elastic scattering of any nucleon in the Fermi sea because all states of the same energy as  $E(k)$  are occupied. If  $\psi$  is analyzed in partial waves, then each of those behaves for large  $x$  like a free particle wave, i.e. there is no phase shift. This property will be important later on.

Comparing (2.9) and (2.2) we see that

$$(k | \tilde{G} | k_0, P) = (2\pi)^{-3} \int d^3 k' (k | \tilde{v} | k') \psi(k'), \quad (2.12)$$

† In the literature, this quantity is normally called  $-e$ .

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where the integral now goes over *all* momentum space. We define the Fourier transform of  $G$ ,

$$G(\mathbf{x}) = (2\pi)^{-3} \int (\mathbf{k} | G | \mathbf{k}_0, \mathbf{P}) e^{i\mathbf{k}\cdot\mathbf{x}} d^3k, \quad (2.13)$$

and that of  $v$  by (2.4). Then (2.12) transforms simply into

$$G(\mathbf{x}) = v(\mathbf{x}) \psi(\mathbf{x}). \quad (2.14)$$

If  $v$  is non-local, then (2.5) yields instead

$$G(\mathbf{x}) = \int d^3y \psi(y) (y | v | \mathbf{x}). \quad (2.15)$$

Equations (2.14) and (2.15) are the standard expressions for the reaction matrix. Inserting (2.13) and (2.14) into (2.10) we find

$$\psi(\mathbf{x}) = e^{i\mathbf{k}_0 \cdot \mathbf{x}} - \int d^3y v(y) \psi(y) \Gamma(\mathbf{x}, \mathbf{y}), \quad (2.16)$$

with the 'non-local operator'  $\Gamma$  defined by

$$\Gamma(\mathbf{x}, \mathbf{y}) = (2\pi)^{-3} \int_{\mathbf{k}_F} \frac{d^3k}{e(k)} e^{i\mathbf{k} \cdot (\mathbf{x} - \mathbf{y})}, \quad (2.17)$$

the integral being taken over the region outside the Fermi sphere. If the interaction  $v$  itself is non-local, (2.16) is replaced by

$$\psi(\mathbf{x}) = e^{i\mathbf{k}_0 \cdot \mathbf{x}} - \int d^3y d^3z (z | v | y) \psi(z) \Gamma(\mathbf{x}, \mathbf{y}). \quad (2.18)$$

If the nucleon energies  $E(k)$  are given,  $\Gamma$  can be calculated from (2.17) by quadrature, and then the integral equation (2.16) can be solved. In particular, if  $v(y)$  contains a repulsive core, (2.6), then for (2.16) to be sensible it is necessary that  $\psi$  vanish inside the core,

$$\psi(\mathbf{x}) = 0 \quad (x < r_c), \quad (2.19)$$

which is the same condition as without exclusion principle. It is important that  $\psi$  was chosen such that  $v(x)$  occurs only multiplied by  $\psi$  at the same position.

For practical solution, it is convenient if the integral equation (2.16) can be transformed into a differential equation. This is possible if  $e(k)$  is a quadratic function of  $k$ . Let us assume, therefore, that

$$E(k) = k^2/2M^*, \quad (2.20)$$

where  $M^*$  is the so-called effective mass (Brueckner 1955a). Then

$$e(k) = (k^2 - k_0^2)/M^* \quad (2.21)$$

independently of  $\mathbf{P}$ . We may then multiply (2.9) by  $e(k)$  which eliminates the  $\delta(\mathbf{k} - \mathbf{k}_0)$ , and then take the Fourier transform. This yields

$$(M^*)^{-1} (\nabla^2 \psi(\mathbf{x}) + k_0^2 \psi(\mathbf{x})) = \int d^3y v(y) \psi(y) \Delta(\mathbf{x} - \mathbf{y}), \quad (2.22)$$

$$\Delta(\mathbf{x} - \mathbf{y}) = (2\pi)^{-3} \int_{\mathbf{k}_F} d^3k e^{i\mathbf{k} \cdot (\mathbf{x} - \mathbf{y})}. \quad (2.23)$$

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Now  $\Delta(\mathbf{x} - \mathbf{y})$  is conveniently broken up into the integral over all momentum space which yields  $\delta(\mathbf{x} - \mathbf{y})$ , minus that over the excluded states

$$g(\mathbf{x} - \mathbf{y}) = (2\pi)^{-3} \int_0^{k_F} d^3 k e^{i\mathbf{k} \cdot (\mathbf{x} - \mathbf{y})}, \quad (2.24)$$

where the integral goes over the region *not* satisfying (2.3).

The Schrödinger equation (2.22) becomes

$$(M^*)^{-1} (\nabla^2 \psi(\mathbf{x}) + k_0^2 \psi(\mathbf{x})) = v(\mathbf{x}) \psi(\mathbf{x}) - \int d^3 y v(\mathbf{y}) \psi(\mathbf{y}) g(\mathbf{x} - \mathbf{y}), \quad (2.25)$$

where the last, non-local term contains the effect of the Pauli principle.

We shall now make the further, quite restrictive, assumption that the centre of mass is at rest,  $\mathbf{P} = 0$ . Then the excluded volume becomes simply a sphere of radius  $k_F$  and (2.24) yields

$$g(x) = \frac{\sin k_F x - k_F x \cos k_F x}{2\pi^2 x^3}. \quad (2.26)$$

This is the well-known formula for the defect in nucleon density due to the exclusion principle, at a distance  $x$  from a fixed nucleon. The exclusion principle term in (2.25) has, of course, the opposite sign of the normal effect of the potential,  $v(\mathbf{x}) \psi(\mathbf{x})$ .

If the assumption  $\mathbf{P} = 0$  is made, then the integro-differential equation (2.25) separates in polar co-ordinates; this will be carried out in the next section. If  $\mathbf{P} \neq 0$ , the expression (2.24) is quite complicated and waves of different angular momenta get mixed.

A possible improvement over (2.20) and (2.21) is the assumption that there is a constant displacement in energy of the occupied as compared with the empty states, caused in part by the 'propagation off the energy shell' (Brueckner 1955*b*, and B, § III). Then  $E$  is given by (2.20) for  $k > k_F$ , but

$$E(k) = k^2/2M^* - \epsilon \quad (k < k_F) \quad (2.27)$$

$$\text{and} \quad \epsilon = (k^2 - k_0^2)/M^* + 2\epsilon. \quad (2.28)$$

The same operations as led to (2.25) give then

$$(M^*)^{-1} (\nabla^2 \psi(\mathbf{x}) + k_0^2 \psi(\mathbf{x})) = 2\epsilon [e^{i\mathbf{k}_0 \cdot \mathbf{x}} - \psi(\mathbf{x})] \\ + v(\mathbf{x}) \psi(\mathbf{x}) - \int d^3 y v(\mathbf{y}) \psi(\mathbf{y}) g(\mathbf{x} - \mathbf{y}). \quad (2.29)$$

The first term on the right-hand side is different from zero only for small  $x$ , inside the range of the potential and slightly beyond, and therefore presents no difficulty of convergence.

The actual dependence of  $E$  on energy is likely to be more complicated than (2.27) (see § 6). Although it is possible to derive integro-differential equations for such cases also, it is probably best to use directly the integral equation (2.16) with an iteration procedure. A solution of (2.29) may be used as starting point. As Brueckner & Wada have pointed out, Schrödinger's variational principle may be useful.

When  $\psi$  has been determined, the required  $G$  is found from the inversion of (2.13). In particular, we are interested in the diagonal element (forward scattering amplitude)

$$\langle \mathbf{k}_0 | G | \mathbf{k}_0, \mathbf{P} \rangle = \int G(\mathbf{x}) e^{-i\mathbf{k}_0 \cdot \mathbf{x}} d^3x, \quad (2.30)$$

where  $G(\mathbf{x})$  is given by (2.14) or (2.15). If there is a repulsive core, one obtains  $G(\mathbf{x})$  inside the core directly, without going through the (then meaningless)  $\psi(\mathbf{x})$  (§ 6).

### 3. EQUATION FOR S STATES

If  $v(x)$  is a spherically symmetric potential, equation (2.25) separates in polar co-ordinates. We consider in particular the case of an  $S$  state, i.e.  $\psi$  is spherically symmetric. We further introduce the dimensionless independent variable

$$\mathbf{r} = k_F \mathbf{x}, \quad (3.1)$$

and write

$$\psi(\mathbf{x}) = u(r)/r. \quad (3.2)$$

Then (2.25) becomes

$$\frac{d^2u}{dr^2} + \frac{k_0^2}{k_F^2} u(r) = \frac{M^* v(r)}{k_F^2} u(r) - \frac{M^*}{k_F^2} r \int \frac{d^3s}{k_F^3} v(s) \frac{u(s)}{s} g(\mathbf{r} - \mathbf{s}), \quad (3.3)$$

where  $\mathbf{s} = k_F \mathbf{y}$ .

We set  $|\mathbf{r} - \mathbf{s}| = z$  so that

$$d^3s = 2\pi \frac{s ds dz dz}{r}. \quad (3.4)$$

Carrying out the integral over  $z$  using (2.24) or (2.26) and setting  $\kappa = k/k_F$ , we obtain for the last integral in (3.3)

$$r \int \frac{d^3s}{k_F^3} \frac{u(s) v(s)}{s} g(\mathbf{r} - \mathbf{s}) = \int ds u(s) v(s) \chi(r, s), \quad (3.5)$$

with

$$\chi(r, s) = \pi^{-1} \int_0^1 dk [\cos \kappa |r - s| - \cos \kappa (r + s)] = \frac{1}{\pi} \left[ \frac{\sin |r - s|}{|r - s|} - \frac{\sin (r + s)}{r + s} \right]. \quad (3.6)$$

The Schrödinger equation (3.3) becomes now

$$\frac{d^2u}{dr^2} + \kappa_0^2 u(r) = \frac{M^*}{k_F^2} \left[ v(r) u(r) - \int ds v(s) u(s) \chi(r, s) \right]. \quad (3.7)$$

The last term is the effect of the exclusion principle.

If there is a repulsive core, the wave function  $u(r)$  must vanish inside it,

$$u(r) = 0 \quad \text{for } r < c = k_F r_c. \quad (3.8)$$

This boundary condition, already discussed in (2.19), is the same as without exclusion principle. At large  $r$ ,  $u$  will automatically go over into the free particle wave function, i.e. there will be no phase shift. This effect of the exclusion principle was derived below equation (2.11) and provides an important check on numerical or analytical solutions of (3.7).

## 4. REPULSIVE CORE ONLY

We shall now assume that the potential consists only of a repulsive core (2.6), so that  $v = 0$  for  $r > c = k_F r_o$ .

This assumption is unphysical but the resulting simplification will make it possible to gain insight into the solution.

It is useful further to introduce the abbreviation

$$w(r) = (M^*/k_F^2) v(r) u(r), \quad (4.1)$$

which, according to (2.14), is closely related to  $G(x)$ .

Inside the repulsive core, we must have  $u(r) = 0$  (equation (3.8)). Outside the core,  $v(r) = 0$  and  $u(r)$  is finite, hence  $w(r) = 0$ . Inside the core, however,  $w(r)$  may be non-vanishing since  $u$  is zero and  $v$  infinite. Indeed, since the left-hand side of (3.7) must vanish for  $r < c$ , the function  $w$  must satisfy the integral equation

$$w(r) = \int ds w(s) \chi(r, s) \quad (r < c). \quad (4.2)$$

Outside the core,  $u \neq 0$ . At  $r = c$ ,  $u$  itself must of course be continuous but  $du/dr$  may be discontinuous. We set  $u'(c + \epsilon) = A$ ,  $(4.3)$

where the constant  $A$  has to be determined so that  $u$  asymptotically has the normalization of  $u_0 = \kappa_0^{-1} \sin \kappa_0 r$ . In order to obtain (4.3) from the differential equation (3.7), we must have

$$w(r) = A \delta(r - c) + w_1(r), \quad (4.4)$$

where  $w_1$  is everywhere finite and differs from zero only for  $r < c$ . Then (4.2) may be rewritten

$$w_1(r) = A \chi(r, c) + \int_0^c ds w_1(s) \chi(r, s). \quad (4.5)$$

If the core radius is not too large, a condition which is satisfied by the 'observed' value  $c = 0.77$ , then equation (4.5) can be solved by iteration. Furthermore, it is then a good approximation to expand  $\chi(r, s)$ , equation (3.6), in powers of  $r$  and  $s$  which gives

$$\chi(r, s) = \frac{2rs}{3\pi} [1 - \frac{1}{10}(r^2 + s^2) + \dots]. \quad (4.6)$$

Inserting into (4.5) and carrying out the iteration gives

$$w_1(r) = \frac{2A}{3\pi} cr \left[ 1 - \frac{1}{10}(r^2 + c^2) + \frac{2c^3}{9\pi} + \dots \right], \quad (4.7)$$

where the last term arises from the integral in (4.5). For  $c = 0.77$ , this last term is only about 0.03 which is essentially negligible. Hence it is sufficient to set  $w_1 = A\chi(r, c)$ . For larger core radii, this would of course no longer be true, and then the integral equation (4.5) can no longer be solved easily by iteration. It should be noted that  $w_1$  has the same sign as the term  $A\delta(r - c)$  in (4.4).

Now we insert our solution for  $w$  into (3.7) for  $r > c$ . We have then in this region

$$\begin{aligned} u'' + \kappa_0^2 u &= - \int ds w(s) \chi(r, s) \\ &= -A \chi(r, c) - \int_0^c ds w_1(s) \chi(r, s) \end{aligned} \quad (4.8)$$

$$= -\frac{2A}{3\pi} cr \left[ 1 - \frac{1}{10}(r^2 + c^2) + \frac{2c^3}{9\pi} + \dots \right], \quad (4.9)$$

if the same approximation is used as in (4.7), namely,  $\chi$  is replaced by (4.6) and  $w_1$  by the first term in (4.7). It is then seen that the whole contribution from  $w_1$  is small of order  $c^3/14$ ; thus it is justified to replace  $w$  by the  $\delta$  function alone.

The use of approximation (4.6) is not well justified for  $r \gg c$  and it is better to use the full expression (3.6) for  $\chi(r, c)$  in (4.8) and neglect the integral in this equation. It is further seen that the right-hand side of (4.8) is negative, i.e. the Pauli principle gives a correction to the repulsive core potential which looks like an attractive potential. The wave function  $u$  is made to curve downwards by this effect.

To solve (4.8), we use the Green function method. The differential equation

$$u'' + \kappa_0^2 u = f(r) \quad (4.10)$$

has the solution

$$u = \kappa_0^{-1} \int_0^r f(s) \sin \kappa_0(r-s) ds. \quad (4.11)$$

In our case,

$$f(r) = A\delta(r-c) - A\chi(r,c). \quad (4.12)$$

Using (3.6), the integral (4.11) is elementary but tedious. We are most interested in the behaviour of  $u$  for large  $r$ . In this limit, we may write

$$u(r) = B \sin \kappa_0 r + C \cos \kappa_0 r. \quad (4.13)$$

Then, with our assumptions (i.e. neglecting  $w_1$  in (4.8)), the constants  $B$  and  $C$  are (dropping the subscript 0 in  $\kappa_0$ )

$$\begin{aligned} B &= \frac{A}{2\pi\kappa} \left( [2\pi - Si(1+\kappa)2c - Si(1-\kappa)2c] \cos \kappa c \right. \\ &\quad \left. + \left[ \ln \frac{1+\kappa}{1-\kappa} + Ci(1+\kappa)2c - Ci(1-\kappa)2c \right] \sin \kappa c \right), \quad (4.14) \end{aligned}$$

$$\begin{aligned} C &= \frac{A}{2\pi\kappa} \left( \left[ \ln \frac{1+\kappa}{1-\kappa} - Ci(1+\kappa)2c + Ci(1-\kappa)2c \right] \cos \kappa c \right. \\ &\quad \left. - [Si(1+\kappa)2c + Si(1-\kappa)2c] \sin \kappa c \right), \quad (4.15) \end{aligned}$$

where  $Si$  and  $Ci$  are defined as in Jahnke-Emde.

Now the asymptotic behaviour of  $u$  should be simply  $\kappa_0^{-1} \sin \kappa_0 r$ , i.e. we should have  $B = 1/\kappa$  and  $C = 0$ . The former can easily be achieved by choice of  $A$ ; the latter condition is clearly not fulfilled for a general value of  $c$ . However, we must remember

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that we have neglected  $w_1$  which is only justified for small values of  $c$ . We therefore expand in a power series in  $c$ , and expect that the lowest powers vanish. Indeed, using

$$\begin{aligned} \text{Ci}(1+\kappa)2c - \text{Ci}(1-\kappa)2c &= \int_{(1-\kappa)2c}^{(1+\kappa)2c} \frac{\cos t}{t} dt \\ &= \ln \frac{1+\kappa}{1-\kappa} - 4c^2\kappa + \frac{4}{3}\kappa(1+\kappa^2)c^4 + \dots, \end{aligned}$$

we easily find that

$$C = \frac{2}{9\pi} Ac^4. \quad (4 \cdot 16)$$

The error due to neglect of  $w_1$  is therefore only of order  $c^4$ , a result which can easily be verified as reasonable. Expansion of (4.14) gives

$$B = \frac{A}{2\pi\kappa} \left\{ 2\pi - c \left( 4 - 2\kappa \ln \frac{1+\kappa}{1-\kappa} \right) - \pi\kappa^2 c^2 + c^3 \left( \frac{8}{3} + 6\kappa^2 - \frac{1}{3}\kappa^3 \ln \frac{1+\kappa}{1-\kappa} \right) + O(c^4) \right\} = \frac{1}{\kappa}, \quad (4 \cdot 17)$$

and therefore  $A$  is  $2\pi$  divided by the curly bracket, or, in first approximation,

$$A = \left[ 1 - \frac{c}{\pi} \left( 2 - \kappa \ln \frac{1+\kappa}{1-\kappa} \right) - \dots \right]^{-1}. \quad (4 \cdot 18)$$

Consider, for example, the case  $\kappa = 0$ , which corresponds to both nucleons being at rest. Then the asymptotic wave function is  $\sin kr/\kappa = r$ , a straight line of unit slope. The constant  $A$  which gives the slope immediately outside the core (equation (4.3)), is greater than unity, as shown by (4.18). This must be so because the effect of the Pauli principle, according to (4.8), is equivalent to an attractive potential and causes a downward curvature of  $u$ . Figure 1 gives a picture of the wave function in this case.

The most important quantity is the diagonal element of the scattering matrix which gives the potential energy. According to (2.13), (2.14), (3.2), (3.1) and (4.1)

$$\begin{aligned} (k_0 | \tilde{G} | k_0) &= \int v(\mathbf{x}) \psi(\mathbf{x}) e^{-ik_0 \cdot \mathbf{x}} d^3x \\ &= \frac{4\pi}{M^* k_F} \int w(r) \frac{\sin \kappa_0 r}{\kappa_0 r} r dr. \end{aligned} \quad (4 \cdot 19)$$

Using (4.4) and neglecting again  $w_1$ ,

$$(k_0 | \tilde{G} | k_0) = \frac{4\pi}{M^* k_F} \frac{A \sin \kappa_0 c}{\kappa_0} = \frac{4\pi A \sin k_0 r_c}{M^* k_0}. \quad (4 \cdot 20)$$

For comparison, we consider the case when the exclusion principle is neglected but the same effective mass is used. Then general scattering theory gives

$$(k_0 | \tilde{G} | k_0) = -\frac{4\pi \tan \delta_0}{M^* k_0}, \quad (4 \cdot 21)$$

where  $\delta_0$  is the phase shift. For a repulsive core,  $\delta_0 = -k_0 r_c$  and

$$(k_0 | \tilde{G} | k_0)_{N,N} = \frac{4\pi \tan k_0 r_c}{M^* k_0}. \quad (4 \cdot 22)$$

Therefore, the ratio of the reaction matrix with and without exclusion principle is

$$\mathcal{R} = \frac{(k_0 | \tilde{G} | k_0)_X}{(k_0 | \tilde{G} | k_0)_{NX}} = A \cos k_0 r_c. \quad (4.23)$$

The effect of a repulsive core is therefore enhanced, owing to the exclusion principle, by the factor  $A \cos k_0 r_c$ . For instance, in the particular case  $k_0 = 0$  (two nucleons at rest), equation (4.14) with (4.23) gives

$$\mathcal{R} = \frac{1}{1 - \pi^{-1} \operatorname{Si} 2c}. \quad (4.24)$$

For  $c = 0.77$ , this is 1.75. Thus the Pauli principle shifts the level  $k_0 = 0$  upward, just as it does for a conventional potential (B, § X). In first approximation, this shift is proportional to  $c$ ,

$$\mathcal{R} \approx A \approx 1 + 2c/\pi. \quad (4.25)$$

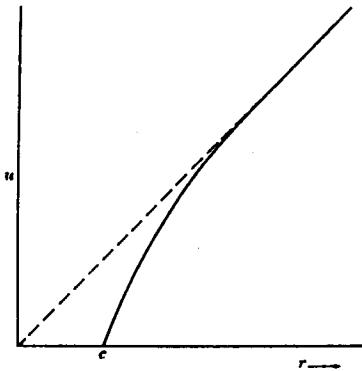


FIGURE 1. Wave function with a pure repulsive core (radius  $c$ ) and the exclusion principle. Note that the asymptote (at large  $r$ ) would pass through the origin.

The maximum of  $A$  (for  $c = \pi$ ) is slightly over 2, for such large  $c$ , however, the neglect of  $w_1$  becomes important, and in general the correct value of  $A$  is greater than (4.24).

For  $\kappa \neq 0$ , i.e. when the two nucleons are not at rest, the correction due to the Pauli principle decreases. Indeed, comparing (4.20), (4.21) and (4.17) we find, to third order in  $c$ :

$$\begin{aligned} \frac{(k_0 | \tilde{G} | k_0)_X}{(k_0 | \tilde{G} | k_0)_{NX}} &= A \cos \kappa c \\ &= \frac{2\pi}{2\pi - c \left( 4 - 2\kappa \ln \frac{1+\kappa}{1-\kappa} \right) + c^3 \left( \frac{8}{3} + 4\kappa^2 + \frac{2}{3}\kappa^3 \ln \frac{1+\kappa}{1-\kappa} \right)}. \end{aligned} \quad (4.26)$$

When  $\kappa = 0.83$ , the coefficient of  $c$  in the denominator vanishes, and for still larger  $\kappa$ , the ratio (4.26) becomes less than one. For  $\kappa$  very near 1, the denominator of (4.14) becomes logarithmically infinite: the  $-C_i(1-\kappa)2c$  contributes  $-\ln(1-\kappa)$  with the same sign as the logarithm occurring explicitly. Thus the interaction  $G$  vanishes if

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the momenta of both nucleons are  $k_F$ , and opposite to each other. However, when the interaction of one nucleon  $k_F$  with all other nucleons is integrated over the momentum of these others, the result will not vanish. In any case, the levels near the top of the Fermi distribution will be shifted *less* upward by the Pauli principle than those near the bottom, or may be shifted slightly downward, as in the example of Brueckner & Wada. The energy spectrum is therefore less spread out, and  $M^*$  is larger than without the Pauli principle.

### 5. ATTRACTIVE POTENTIAL

If there is only an attractive potential (no repulsive core), e.g. a square well, then equation (3.7) shows that there is one region of  $r$  (that of the well itself) in which the main effect is that of the attractive potential itself (first term on the right of (3.7)) and another region, just outside the well, in which the second (Pauli principle) term of (3.7) dominates which has, in this case, the same effect as a repulsive potential. These two opposing effects are necessary in order to make the wave function  $u$  asymptotically equal to that of a free particle, without any phase shift.

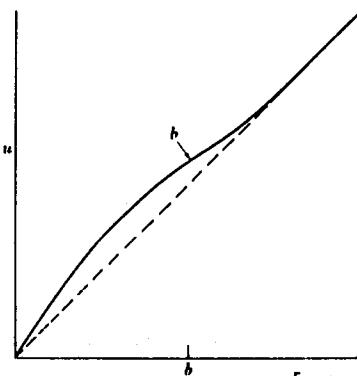


FIGURE 2. Wave function for a pure attractive potential. Radius of interaction  $b$ . The wave function (solid line) stays close to the free particle function  $u = r$  (dashed line).

The behaviour of the wave function  $u$  for  $\kappa_0 = 0$  is shown schematically in figure 2. The curvature is first downward, then upward, and the wave function never deviates very much from the straight line  $u = r$  which would hold for a free particle. The reaction matrix (4.19) is therefore not very different from the result obtained if  $u$  were replaced by  $r$ , i.e. from the Born approximation. The correct result is slightly larger than this since  $u > r$  (figure 2). This result is just the same as was derived in B, § X: the Born approximation should be very good but slightly too small. We have here shown how this result manifests itself in the spatial wave function.

If there is a repulsive core and an attractive potential, the quasi-attractive Pauli term due to the core (see equation (4.8)) and the main term due to the attractive potential will occur in the same range of  $r$ , followed by a quasi-repulsive Pauli term, from the attractive potential, at larger  $r$ . The wave function may have approximately

the form of figure 3. Through most of the region of the attractive potential,  $u$  will be less than the free wave function  $r$  (for  $\kappa_0 = 0$ ) but  $u$  will always be greater than

$$u_s = \frac{b}{b-c} (r - c), \quad (5.1)$$

where  $b = k_F r_a$  and  $r_a$  is the outer edge of the attractive well. This makes it possible to give a lower and a (probable) upper limit to the contribution of the attractive potential to the reaction matrix (4.19), which are fairly close.

The effect of the repulsive core is more difficult to estimate because it depends on the slope of the wave function  $u$  just outside the core, rather than on an integral over  $u$ .

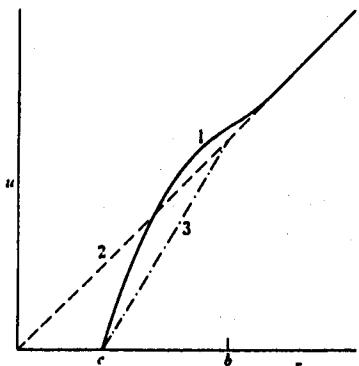


FIGURE 3. Wave function for a repulsive core (radius  $c$ ) plus attractive potential (radius  $b$ ), using the exclusion principle. The straight line 2 is a rough upper limit, the line 3 a rigorous lower limit for the actual wave function, curve 1.

To obtain the reaction matrix  $G$  quantitatively, it is necessary to solve the wave equation (2.25) or (2.16) more accurately. Probably, a variational principle such as that used by Brueckner & Wada will be useful. These authors have used as trial wave functions those obtained without the Pauli principle which do have a phase shift at infinity. A qualitative knowledge of the form of the actual wave function, as derived in this paper, should lead to a better trial function.

The effective mass enters equation (3.7) as a factor multiplying the potential. The smaller  $M^*$ , the nearer will the reaction matrix for an attractive potential be to that of the Born approximation. For larger  $M^*$ , the  $G$  for an attractive potential will increase. Both of these results are opposite to those for a repulsive core, equation (4.20). However, repulsive and attractive potential have in common that the energy levels of the nucleons are raised by reducing  $M^*$ . The reaction matrix  $G$  itself is a difference between two large terms, a positive term from the repulsive core and a negative one from the attractive well outside. But a decrease of  $M^*$  will make both of them more positive. Hence the result is very sensitive to the choice of  $M^*$ , as has been pointed out by Brueckner. This probably means also that the effective-mass approximation itself is not sufficiently accurate.

## 6. EFFECTIVE MASS

Brueckner & Wada have carried out their calculation in the effective-mass approximation, fixing the effective mass by the condition

$$E(k_F) - E(0) = k_F^2/2M^*, \quad (6.1)$$

i.e. the energy of occupied states is fitted on the average. Since the transitions are all to empty states, a fit at somewhat larger  $k$  may be preferable. We want to investigate here the region of very large  $k$ , and in particular whether the effective mass principle is applicable in this region at all, i.e. whether the energy is quadratic in  $k$ .

We consider two nucleons of initial momenta  $\mathbf{k}_1, \mathbf{k}_2$  inside the Fermi sphere. By a collision, they may go to an intermediate state  $\mathbf{k}'_1 = \mathbf{k}_1 + 2\mathbf{k}, \mathbf{k}'_2 = \mathbf{k}_2 - 2\mathbf{k}$  (the factor 2 is inserted for convenience in the following). We assume that  $2k \gg k_F$ , then  $\mathbf{k}_1$  and  $\mathbf{k}_2$  may be neglected and we have two nucleons of momenta  $+2\mathbf{k}$  and  $-2\mathbf{k}$ . We now have to calculate the interaction of each of these nucleons with all the nucleons remaining in the Fermi sea, e.g. with one of momentum  $\mathbf{k}_3$ . For this purpose, we again have to solve the integral equation for the scattering matrix, for the scattering of the nucleon  $2\mathbf{k}$  by the nucleon  $\mathbf{k}_3$  and we may again neglect  $\mathbf{k}_3$  compared with  $2\mathbf{k}$ . Then the intermediate states in this scattering will have the nucleons 1 and 3 at the momenta

$$\mathbf{k}''_1 = \mathbf{k} + \mathbf{q}, \quad \mathbf{k}''_3 = \mathbf{k} - \mathbf{q}, \quad (6.2)$$

while nucleon 2 remains at  $\mathbf{k}_2 = -2\mathbf{k}$ . As shown in B, equation (3.7), the energy denominator is, then, the sum of the excitation energies of all three nucleons, i.e. (neglecting initial energies)

$$e = E(\mathbf{k} + \mathbf{q}) + E(\mathbf{k} - \mathbf{q}) + E(-2\mathbf{k}), \quad (6.3)$$

and in the notation of B, equation (3.7).

$$\begin{aligned} (\mathbf{k}'_1 \mathbf{k}_3 | \tilde{G} | \mathbf{k}'_1 \mathbf{k}_3; \mathbf{k}_1 \mathbf{k}_2, \mathbf{k}'_2) &= (\mathbf{k}'_1 \mathbf{k}_3 | \tilde{v} | \mathbf{k}'_1 \mathbf{k}_3) \\ &- (2\pi)^{-3} \int d^3 k'' (\mathbf{k}'_1 \mathbf{k}_3 | \tilde{v} | \mathbf{k}''_1 \mathbf{k}''_3) (1/e) (\mathbf{k}''_1 \mathbf{k}''_3 | \tilde{G} | \mathbf{k}'_1 \mathbf{k}_3; \mathbf{k}_1 \mathbf{k}_2, \mathbf{k}'_2). \end{aligned} \quad (6.4)$$

We shall now assume that the energy is proportional to  $k^2$  for large  $k$ , i.e. that (2.20) is valid, and calculate  $G$  and  $V(k)$  (B, equation 9.14). We shall find that the resulting  $V(k)$  is indeed proportional to  $k^2$ : this calculation will of course also yield the value of  $M^*$ . The potential will be taken as a local potential  $v(x)$  and will be assumed to contain a repulsive core (2.6). We use the spatial wave function (2.10): in our notation,  $\mathbf{k}_0$  is to be replaced by  $\mathbf{k}$  and  $\mathbf{k}$  of (2.10) by  $\mathbf{q}$ . Inserting  $e$  from (6.3) and (2.20), we have then

$$\psi(\mathbf{x}) = e^{i\mathbf{k} \cdot \mathbf{x}} - \frac{M^*}{(2\pi)^3} \int \frac{(\mathbf{q} | \tilde{G} | \mathbf{k}, \mathbf{k})}{3k^2 + q^2} e^{i\mathbf{q} \cdot \mathbf{x}} d^3 q. \quad (6.5)$$

Equation (2.16) is then valid with

$$\Gamma(x, y) = \frac{M^*}{(2\pi)^3} \int_{|\mathbf{q}| \pm k \approx k} \frac{d^3 q}{3k^2 + q^2} e^{i\mathbf{q} \cdot (\mathbf{x} - \mathbf{y})}. \quad (6.6)$$

The energy denominators are again positive definite: this time this is not due to the Pauli principle but to the 'propagation off the energy shell', i.e. to the fact that all energies in (6.3) are counted from the normally occupied states  $\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3$  (rather than from  $\mathbf{k}'_1, \mathbf{k}'_2, \mathbf{k}'_3$ ). Owing to the Pauli principle, the momentum of the nucleon  $\mathbf{k}_3$  after collision, which according to our assumptions is  $\mathbf{q} - \mathbf{k}$ , must be greater than  $\mathbf{k}_F$ ; also  $|\mathbf{k} + \mathbf{q}| > k_F$ .

It is convenient to transform to a differential equation. Using (2.24), we find from (6.6)

$$(\nabla_x^2 - 3k^2) \Gamma(x, y) = -M^*[\delta(\mathbf{x} - \mathbf{y}) - 2 \cos \mathbf{k} \cdot (\mathbf{x} - \mathbf{y}) g(\mathbf{x} - \mathbf{y})], \quad (6.7)$$

where  $\nabla_x^2$  denotes the Laplacian in  $\mathbf{x}$  space. Inserting into (2.16) yields

$$(\nabla^2 - 3k^2) \psi(\mathbf{x}) = -4k^2 e^{ik \cdot \mathbf{x}} + M^* \left[ v(\mathbf{x}) \psi(\mathbf{x}) - \int d^3 y 2 \cos \mathbf{k} \cdot (\mathbf{x} - \mathbf{y}) g(\mathbf{x} - \mathbf{y}) v(\mathbf{y}) \psi(\mathbf{y}) \right]. \quad (6.8)$$

Inside the core,  $\psi = 0$ ; therefore, if we disregard effects at the surface of the core (which will be discussed below), the right-hand side must vanish. The solution is obtained by the same method as in § 4 and is

$$M^* v(\mathbf{x}) \psi(\mathbf{x}) = 4k^2 e^{ik \cdot \mathbf{x}} [1 + (4/9\pi) c^3 + \dots], \quad (6.9)$$

where the term in  $c^3$  arises from the Pauli principle. This term, and generally the last term in (6.8), will be neglected in the following.

To solve (6.8) near the surface of the core ( $r = r_c$ ), we assume  $kr_c \gg 1$ : then the surface may be considered as plane, and defined as the plane  $z = 0$  (positive  $z$  = outside core). Then if  $\theta$  is the angle between  $\mathbf{k}$  and the  $z$  axis.

$$\exp(ik \cdot \mathbf{x}) = \exp ik [(r_c + z) \cos \theta + x \sin \theta], \quad (6.10)$$

$$v = v_0 \rightarrow \infty \quad \text{for } z < 0, \quad v = 0 \quad \text{for } z > 0, \quad (6.11)$$

and we set

$$\psi = \exp(ik z \sin \theta) \phi(z). \quad (6.12)$$

The equation for  $\phi$  is

$$\phi'' - k^2(3 + \sin^2 \theta) \phi = -4k^2 e^{ik \cos \theta (r_c + z)} + M^* v(z) \phi(z). \quad (6.13)$$

For  $z > 0$ , since  $v = 0$ , the solution is

$$\phi = (e^{ikz \cos \theta} - e^{-Kz}) e^{ikr_c \cos \theta}, \quad (6.14)$$

$$K = (3 + \sin^2 \theta)^{1/2} k. \quad (6.15)$$

In (6.14), we have made use of the fact that  $\phi$  must vanish at the surface of the core,  $z = 0$ . Inside the core  $M^* v \phi$  consists of two parts, the volume term (6.9) and a  $\delta$  function at the surface, similar to § 4,

$$M^* v \phi = 4k^2 e^{ik \cos \theta (r_c + z)} + C \delta(z). \quad (6.16)$$

The volume term alone gives a negligible  $\phi$  and  $\phi'$ . The surface term gives a jump of  $\phi'$  from 0 at  $z = -\epsilon$  to

$$\phi' = C = (K + ik \cos \theta) e^{ikr_c \cos \theta} \quad (6.17)$$

at  $z = +\epsilon$ , using (6.14).

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The reaction matrix is given by (2.30), with  $k_0$  replaced by  $k$ . Inserting (6.16) (6.17) we get

$$\langle \mathbf{k} | \tilde{G} | \mathbf{k}, \mathbf{k} \rangle = \int_{r_c}^{r_c} [4k^2 + (K + ik \cos \theta) \delta(r - r_c)] d^3r. \quad (6.18)$$

Both volume and surface term are independent of the strength of the repulsive potential. The integral goes over the volume of the core and gives

$$\begin{aligned} \langle \mathbf{k} | \tilde{G} | \mathbf{k}, \mathbf{k} \rangle &= \frac{4\pi}{M^*} \left[ \frac{4}{3} k^2 r_c^3 + k r_c^2 \left( \frac{\pi}{3} + \frac{\sqrt{3}}{2} \right) \right] \\ &= \frac{16\pi}{3M^*} r_c^2 [k^2 r_c + 1.430k]. \end{aligned} \quad (6.19)$$

The first (volume) term is proportional to  $k^2$ , in accord with the effective mass assumption, and therefore justifies this assumption for high momenta in the case of a hard core. The second (surface) term in (6.19) is proportional to  $k$  which also follows from dimensional considerations. The term  $C\delta(r - r_c)$  from which this surface contribution arises, is the closest analogue to the main term  $A\delta(r - c)$  at low energy (equation (4.4)). The term proportional to  $k$  in (6.19) has the consequence that  $G$  depends on  $k$  more strongly at low  $k$  than the effective mass approximation would indicate, i.e. that the 'effective mass' is smaller for low  $k$  than for high. The linear term is very large: only for  $2k > 3/r_c$  will the quadratic term in (6.19) dominate.

The potential energy of a nucleon in state  $\mathbf{k}'_1$  is obtained by integrating over all nucleons  $\mathbf{k}_3$  in the Fermi distribution (see beginning of this section), namely,

$$V(k'_1) = 4(2\pi)^{-3} \int d^3k_3 \langle \mathbf{k}'_1, \mathbf{k}_3 | \tilde{G} | \mathbf{k}'_1, \mathbf{k}_3 \rangle. \quad (6.20)$$

The factor 4 has been used rather than the 3 of B, equation (9.14), because we are now using an ordinary rather than a Serber potential so that the interaction between two particles of equal spin is no longer zero, in contrast to B, equation (8.23). (We are neglecting the exchange terms in B, equations (8.14) to (8.18).) Now  $\tilde{G}$  in (6.20) is the same as in (6.19) and is independent of  $k_3$ . The integral over  $\mathbf{k}_3$  then gives simply the nucleon density (B, equation 9.11) and

$$V(2k) = \frac{\tilde{G}}{(4\pi/3) r_0^3} = \frac{4r_0^2}{M^* r_0^3} [k^2 r_c + 1.430k], \quad (6.21)$$

where  $r_0 A^{\frac{1}{3}}$  is the nuclear radius (cf. B, equation (9.12)). Neglecting the term proportional to  $k$ , the total energy is then

$$\begin{aligned} E(2k) &= V(2k) + \frac{4k^2}{2M} \\ &= 4k^2 \left( \frac{r_c^3}{M^* r_0^3} + \frac{1}{2M} \right) \equiv \frac{4k^2}{2M^*}. \end{aligned} \quad (6.22)$$

from which

$$M^* = M \left( 1 - \frac{2r_c^3}{r_0^3} \right). \quad (6.23)$$

Putting  $r_0 = 1.18 \times 10^{-13}$  according to B, equation (9.12), and choosing

$$r_c = 0.6 \times 10^{-13}$$

according to (2.7) we get

$$M^* = 0.74M, \quad (6.24)$$

which is not too far from the value found by Brueckner & Wada at low energy,  $M^* = 0.60M$ . However, there are strong indications that the repulsive core has a much smaller radius than (2.7) in states of isotropic spin 0 of the two-nucleon system (or maybe in triplet states). Taking  $r_c = 0.5 \times 10^{-13}$  as an average, we get

$$M^* = 0.85M. \quad (6.25)$$

Then there is a considerable increase of the effective mass with energy, and substantial corrections to the effective mass approximation will be required.

We have assumed that the repulsive core acts equally in all states. If it acted only in  $s$  states (which is an unlikely assumption) the interaction  $V(k)$  would be reduced by a factor of the order  $(kr_c)^{-1}$ . It would thus become independent of  $k$ , which would mean that the effective mass would then be equal to the actual mass  $M$ , and at high  $k$  there would merely be a constant shift in energy as compared with free particles.

*Note added in proof, 10 December 1956.* The interpretation of the calculation of §6 as giving the effective mass is not correct. This is because the energy  $E(k'_1)$  has no significance by itself but is required in order to calculate the excitation energy

$$\Delta = E(k'_1) + E(k'_3) - E(k_1) - E(k_3). \quad (6.26)$$

Each of the energies in (6.26) is obtained by integrating the scattering matrix  $G$  for the interaction of the respective nucleon with all other nucleons  $k_s$ , as in (6.20). Now to calculate the scattering matrix for  $k_1$ , one must assume that the two nucleons  $k'_1, k'_3$  remain in the field (Goldstone 1957); the energy denominator for the calculation of  $G(k_1, k_3)$  is

$$\bar{e} = E(k'_1) + E(k'_3) - E(k_1) - E(k_3) + \Delta \quad (6.27)$$

Because of the appearance of  $\Delta \approx 4k^2/M^*$  this is nearly the same as the denominator  $(3k^2 + q^2)/M^*$  in (6.5). The only difference is then in the influence of the Pauli principle which should be somewhat greater in  $G(k_1 k_3)$  than in  $G(k'_1 k'_3)$ . The main term (6.21) will be cancelled by a similar term in  $E(k_1)$ , and only perhaps 10 per cent of this amount will remain. Thus the effective mass will actually be very close to  $M$ , a conclusion which is physically more reasonable than that reached above.

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**Neutron Star Matter**  
(with G. Baym and C. J. Pethick)  
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When, in 1968, pulsars were discovered, and interpreted as rotating neutron stars, I turned my attention again to astrophysics. In this paper, the equation of state pertinent to a neutron star is calculated, as a function of density and of the fraction of neutrons. Many refinements were later introduced. The most recent is the condensation of  $K^-$  mesons in nuclear matter of density above about 3 times normal nuclear density.

## NEUTRON STAR MATTER

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**Abstract:** The matter in neutron stars is essentially in its ground state and ranges in density up to and beyond  $3 \times 10^{14} \text{ g/cm}^3$ , the density of nuclear matter. Here we determine the constitution of the ground-state of matter and its equation of state in the regime from  $4.3 \times 10^{11} \text{ g/cm}^3$  where free neutrons begin to "drip" out of the nuclei, up to densities  $\approx 5 \times 10^{14} \text{ g/cm}^3$ , where standard nuclear-matter theory is still reliable. We describe the energy of nuclei in the free neutron regime by a compressible liquid-drop model designed to take into account three important features: (i) as the density increases, the bulk nuclear matter inside the nuclei, and the pure neutron gas outside the nuclei become more and more alike; (ii) the presence of the neutron gas reduces the nuclear surface energy; and (iii) the Coulomb interaction between nuclei, which keeps the nuclei in a lattice, becomes significant as the spacing between nuclei becomes comparable to the nuclear radius. We find that nuclei survive in the matter up to a density  $\sim 2.4 \times 10^{14} \text{ g/cm}^3$ ; below this point we find no tendency for the protons to leave the nuclei. The transition between the phase with nuclei and the liquid phase at higher densities occurs as follows. The nuclei grow in size until they begin to touch; the remaining density inhomogeneity smooths out with increasing density until it disappears at about  $3 \times 10^{14} \text{ g/cm}^3$  in a first-order transition. It is shown that the uniform liquid is unstable against density fluctuations below this density; the wavelength of the most unstable density fluctuation is close to the limiting lattice constant in the nuclear phase.

### 1. Introduction

The identification of pulsars as rotating neutron stars <sup>1)</sup> has renewed interest in the properties of matter at very high densities. The density of matter in a neutron star increases with depth from low values near the surface to central densities on the order of the density of matter in nuclei ( $\approx 0.2 \text{ nucleons/fm}^3$  or  $3 \times 10^{14} \text{ g/cm}^3$ ) or greater. Except in the outermost layer of a neutron star, the matter is relatively very cold in the sense that characteristic energies required for microscopic excitations are very much greater than the characteristic thermal energy,  $k_B T$ . If the matter has had sufficient time in the earlier hot stages of the star to reach nuclear equilibrium, one may consider it to be in its absolute ground state. This requires that nuclear equilibration rates be fast compared with cooling rates.

Up to a mass density  $\rho \sim 10^7 \text{ g/cm}^3$ , the ground state of matter consists of <sup>56</sup>Fe nuclei arranged in a lattice, most likely body-centered cubic (bcc), together with a

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sea of electrons<sup>2,3,4</sup>). Beyond  $\rho \sim 10^3 \text{ g/cm}^3$  the electrons are fully ionized, and above  $\sim 10^6 \text{ g/cm}^3$  they are relativistic and virtually free. As the density of matter rises, with increasing depth in the star, the equilibrium nucleus present becomes more and more neutron rich, as a result of electron capture. The binding energy of the last neutron in the equilibrium nucleus becomes smaller, and eventually, at a density<sup>4</sup>)  $\rho_d = 4.3 \times 10^{11} \text{ g/cm}^3$ , it becomes favorable for neutrons to begin to "drip" out of the nuclei. At densities between  $\rho_d$  and  $\rho \sim 2.4 \times 10^{14} \text{ g/cm}^3$ , the matter is still solid, and consists of a lattice of nuclei immersed in a pure neutron gas, in addition to the electron gas; we shall refer to this regime as the *free neutron regime*. The nuclei dissolve at about nuclear matter density and at higher densities the matter consists of a uniform liquid of neutrons with a small fraction of protons and electrons. As we shall see, muons also appear at about this point. Finally, at densities a few times higher, various hyperons,  $\Sigma^-$ ,  $\Lambda^0$ , etc., make their appearance.

In this paper we shall be concerned with determining the nuclei present in the free neutron regime, as well as the properties of the liquid phase, the nature of the transition between these two phases, and the equation of state of the matter in these phases. The calculations given here are for densities below  $\approx 5 \times 10^{14} \text{ g/cm}^3$ , beyond which the usual techniques of nuclear matter theory require modification.

In two recent papers<sup>5,6</sup>) on the properties of the free neutron regime, the semi-empirical mass formula<sup>7</sup>) was used to describe the nuclear energies. The dissolving of the nuclei was found in both these papers to take place at  $\rho \approx 5 \times 10^{13} \text{ g/cm}^3$ . We have found on closer examination that this result is very sensitive to the particular description used for the neutron gas surrounding the nuclei; in ref.<sup>5</sup>), the Nemeth-Sprung "la" description<sup>8</sup>), and in ref.<sup>6</sup>), a description based on a Levinger-Simmons potential were used. In particular when more accurate calculations of the properties of neutron matter are used, one finds the curious result that it is impossible to construct a thermodynamically consistent picture of the dissolving of the nuclei. Both  $\mu_n$ , the neutron chemical potential (equal to minus the separation energy) and the pressure  $P$  must be continuous through the transition. The inconsistency arises from the fact that according to the semi-empirical mass formula,  $\mu_n$  must always be less than  $\approx 8.3 \text{ MeV}$  for the nuclei present. This number is a sum of  $\approx -16 \text{ MeV}$  volume energy and  $\approx 24 \text{ MeV}$  symmetry energy; surface and Coulomb terms contribute  $\sim 5\%$  of the total. However, the pressure in the nuclear phase is always *higher* than that for the liquid phase at the same  $\mu_n$ . The nuclear phase remains thermodynamically preferable; there is no way to have both  $\mu_n$  and  $P$  continuous across the transition. This limitation on  $\mu_n$  is clearly unphysical, and is due to the use of the semi-empirical mass formula in the region of very neutron-rich nuclei, for which it is not designed.

One important physical feature not taken into account in the semi-empirical mass formula is that the matter inside very neutron-rich nuclei is quite similar to both the pure neutron gas outside the nuclei, as well as to the neutron matter in the uniform liquid state. However, the bulk terms in the usual semi-empirical mass formula

describe this matter very differently from the calculations one uses for the neutron matter. In the present work we shall remove this inconsistency by using a single expression for the energy of bulk nuclear matter, as a function of density and proton concentration, to describe both the nuclear matter in nuclei, the neutron gas outside, and the uniform liquid state. As a result we shall find that it is possible to have co-existence of bulk nuclear matter with a pure neutron gas up to  $\mu_n \sim 30$  MeV (compared with the  $\approx 8.3$  MeV result earlier); this allows us to develop a consistent picture of the transition.

A second important physical effect not taken into account in the earlier work is the attractive Coulomb interaction between nuclei – the ordinary solid-state lattice binding energy. The optimal nuclear size in neutron star matter is determined by a delicate balance between nuclear Coulomb and surface energies; the surface energy favors nuclei with a large number of nucleons,  $A$ , while the nuclear Coulomb self-energy, that of protons within a nucleus, favors small nuclei. The lattice energy, of similar structure to the Coulomb self-energy, but of opposite sign, favors large nuclei. When the lattice energy begins to become comparable in magnitude with the nuclear Coulomb self-energy, that is, when the nuclear radius becomes comparable with the spacing between nuclei, the effect on the equilibrium value of  $A$  becomes considerable. For example, when neutron drip first sets in, inclusion of the lattice energy raises  $A$  by  $\sim 15\%$ . At much higher densities the effect is dominant and can no longer be treated as a perturbation. Indeed, were the nuclei to fill all of space, the total Coulomb energy would vanish, since the uniform electron distribution would exactly compensate the uniform proton distribution. It is vital then to include the lattice Coulomb energy in order to have a consistent description of the matter at densities approaching that of nuclear matter. In addition, the lattice energy, by favoring the existence of nuclei, tends to raise the maximum density at which nuclei can exist.

The third physical feature that requires a more careful treatment in the free neutron regime is the nuclear surface energy. One expects the presence of the outside neutron gas to reduce the surface energy, since as the density of the system increases the inside and outside matter become more and more alike; were they the same there would of course be no surface energy. The semi-empirical mass formula takes no account of this reduction of the surface energy. In ref.<sup>3)</sup> it was estimated that this reduction would be only  $\sim 15\%$ , but this was because the transition was thought to be at a much lower density than we find here. At higher mass densities the effect is very large; the reduction of the surface energy lowers the energy of the nuclear phase and thus in turn also raises the maximum density at which nuclei can be present.

Furthermore, the pressure of the neutron gas to which the nuclei are exposed is now sufficiently high that its effect on the nuclei cannot be treated as a perturbation, as was done in ref.<sup>5)</sup>. To remedy these various difficulties with the semi-empirical mass formula we describe the nuclei by a *compressible liquid-drop model*<sup>†</sup> which has

<sup>†</sup> Generalizations in this spirit of the semi-empirical mass formula for ordinary nuclei with no external neutron gas have been given by Myers and Swiatecki<sup>9)</sup> and Weiss and Cameron<sup>10)</sup>.

the following features:

- (i) The nucleus is pictured as a drop of compressible nuclear matter with a well-defined surface; unlike in the semi-empirical mass formula the density of the matter inside the nucleus is treated as a variable, determined by equating the pressure of the nucleus to the outside neutron gas pressure.
- (ii) The energy of the nucleus we take to be a sum of a volume energy, given by the same energy function used to describe the neutron matter; a Coulomb energy, including the lattice energy; and a surface energy appropriately modified by the presence of the outside neutron gas.
- (iii) The parameters of the model are chosen to give reasonable fits to masses of observed nuclei. These energies depend on the density of the interior matter, on  $A$ , the total nucleon number, and  $Z$ , the total proton number, and, in the case of the surface energy, on the outside neutron gas density as well.

We shall treat  $A$  and  $Z$  as continuous variables and neglect shell effects and possible deformations of the nuclei. We shall also neglect pairing effects both in the nuclei and the neutron matter.

The most important conclusion of our work is that nuclei are present in neutron star matter up to mass densities on the order of symmetric nuclear matter density ( $3 \times 10^{14} \text{ gm/cm}^3$ ), some 4–5 times higher than predicted by the earlier calculations [refs. 5, 6)]. This rather large difference comes about since the effects we have taken into account here encourage the formation of nuclei, and they all become increasingly important as the density is increased. An important consequence of this for the structure of neutron stars is that the crust can be much thicker than previously thought and in fact, there can exist completely solid stable neutron stars <sup>4)</sup>. The crust is also capable of storing substantially more elastic energy than previously believed <sup>11)</sup>.

We find that as the matter density increases,  $Z$ , the number of protons per nucleus, increases rather slowly from about 40 at neutron drip to about 100 at  $\rho \sim 10^{14} \text{ g/cm}^3$ , and then increases rapidly to several hundred by the transition. On the other hand the nucleon number  $A$  increases steadily with increasing mass density, starting at  $\sim 120$  at neutron drip, increasing to  $\sim 700$  at  $\rho \sim 10^{14} \text{ g/cm}^3$ ; near the transition where the nuclei dissolve the proton concentration in nuclei is about 5 %, only slightly above that in the uniform liquid.

The structure of this paper is the following. In sect. 2 we derive the general equilibrium conditions that determine the type and density of nuclei present in the free neutron regime. To evaluate these conditions we need an expression for the energy of nuclei immersed in a free neutron sea, as well as the energy of bulk neutron matter. The nuclear energy formula is developed in sects. 3, 4 and 5. In sect. 3 we construct an expression for the energy of bulk nuclear matter as a function of density and proton concentration; for zero proton concentration this expression gives the energy of pure neutron matter. We also discuss here the coexistence between bulk nuclear matter and a pure neutron gas. Sect. 4 is devoted to the nuclear surface energy while in sect. 5 we discuss the Coulomb energy.

With the resulting nuclear mass formula we carry out, in sect. 6, an explicit evaluation of the properties of the free neutron regime. In sect. 7 we consider the possibility of protons also dripping from the nuclei, and conclude that this is unlikely to occur. In sect. 8 we determine the properties of the uniform liquid, and in sect. 9 we discuss the instability of this liquid against proton clustering, and the nature of the transition between the phase with nuclei and the uniform liquid. Finally, sect. 10 contains a discussion of the equation of state of the matter in neutron stars.

## 2. Equilibrium conditions

In the free neutron regime ( $4.3 \times 10^{11} \text{ g/cm}^3 \leq \rho \leq 2.5 \times 10^{14} \text{ g/cm}^3$ ) the matter consists of a lattice of nuclei immersed in neutron and electron seas. Free protons do not appear, except possibly just before the nuclei dissolve. In this section we construct an expression for the total energy of the system, and derive the conditions that determine, at any given matter density in complete nuclear equilibrium at zero temperature, the type of nucleus present and the relative numbers of nuclei and free neutrons.

We picture the nucleus as having a well-defined surface; nucleons within this surface we associate with the nucleus. We let  $Z$  be the total number of protons within the surface and  $A$  the total number of nucleons within the surface. The energy <sup>†</sup>  $W_N(A, Z, V_N, n_n)$  of a given nucleus in the matter depends on  $A$  and  $Z$ , as well as on the number density  $n_n$  of the neutron gas *outside* the nucleus and the volume  $V_N$  of the nucleus.  $W_N$  is taken to include the rest mass of the nucleons. The outside neutrons affect the energy of the nuclei both by modifying the nuclear surface energy and by exerting a pressure on the nuclei; the pressure tends to decrease the nuclear volume, while the modification of the surface energy has the opposite effect. (Nuclei in ordinary matter have zero pressure on their surfaces.) For this reason the nuclear volume must be considered a variable.

We assume the neutron gas outside the nuclei to be uniform and of density

$$n_n = \frac{N_n}{V - N_N V_N}, \quad (2.1)$$

where  $N_n$  is the total number of neutrons outside nuclei, in a volume  $V$ , and  $N_N$  is the total number of nuclei in that volume;  $V - N_N V_N$  is thus the total volume outside the nuclei. We denote by  $E_n(n_n)$  the energy (including rest masses) of the neutron gas per unit volume occupied. Because electron screening lengths are relatively large, the electrons completely penetrate the nuclei and have a uniform density  $n_e$  throughout. Charge neutrality implies that

$$n_e = \frac{Z N_N}{V} \equiv Z n_N \quad (2.2)$$

<sup>†</sup> We shall use the subscript  $N$  to refer to nuclei and  $n$  to neutrons; the letter  $W$  shall denote energies, while the letter  $E$  shall denote energies per unit volume.

as long as all the protons are in nuclei, and no muons are present. The energy density  $E_e(n_e)$  of the electrons is, to within terms of order  $Z^3 e^2/hc$ , just the energy of a free electron gas.

Finally, we must take into account Coulomb interactions between nuclei immersed in a uniform background of electrons. This "lattice" energy, denoted by  $W_L$  per nucleus, is negative and for a body-centered cubic (bcc) lattice, for example, is given by<sup>12)</sup>

$$W_L = -\frac{1.82Z^2e^2}{a}, \quad (2.3)$$

where  $a = (2/n_N)^{1/3}$  is the lattice constant; thus when  $a$  is  $\sim r_N$ , the nuclear radius, this energy is of the same order as the Coulomb energy,  $\approx \frac{2}{3}(Z^2e^2/r_N)$ , of an individual nucleus. In particular, if one imagines the nuclei filling all of space, then both the protons and electrons are uniformly distributed, and the *total* Coulomb energy, nuclear plus lattice, must vanish. The lattice energy thus plays a crucial role in determining the type of nuclei present. At higher densities,  $\gtrsim 10^{14} \text{ g/cm}^3$ , the corrections to (2.3) due to the finite size of the nucleus become important; these will be considered in sect. 5. It should be emphasized that the lattice energy is not an effect peculiar to the solid state; it is only a few percent smaller in magnitude for a liquid<sup>13)</sup>.

The total energy per unit volume of the system, including all rest masses, is then

$$E_{\text{tot}}(A, Z, n_N, V_N, n_n) = n_N(W_N + W_L) + (1 - V_N n_N)E_N(n_n) + E_e(n_e). \quad (2.4)$$

The factor  $1 - V_N n_N$  is the fraction of the total volume occupied by the neutron gas.

The equilibrium conditions for determining  $A$ ,  $Z$ ,  $n_N$ ,  $V_N$  and  $n_n$  at a given mean density  $n_b$  of baryons,

$$n_b = A n_N + (1 - V_N n_N) n_n, \quad (2.5)$$

are derived by minimizing  $E_{\text{tot}}$  with respect to its arguments, keeping  $n_b$  fixed. This leads to four independent conditions, which we now discuss. Consider first the determination of the optimal number of nucleons in a nucleus. Let us ask the question: given, in a unit volume, a certain number  $n_N Z$  of protons and  $n_N(A-Z)$  of neutrons in nuclei, a fixed total fraction  $n_N V_N$  of the volume occupied by nuclei, and a fixed number of neutrons outside the nuclei, what is the optimal  $A$ ? This is determined by minimizing  $E_{\text{tot}}$  with respect to  $A$  at fixed  $n_N A$ ,  $n_N Z$ ,  $n_n$  and  $n_N V_N$ . In this variation  $n_e$ , and the free neutron energy are unaltered, and the resulting condition is simply

$$\frac{\partial}{\partial A} \left( \frac{W_N + W_L}{A} \right)_{x, n_N A, n_N V_N, n_n} = 0, \quad (2.6)$$

where

$$x = \frac{Z}{A} \quad (2.7)$$

is the fractional concentration of protons in nuclei. Eq. (2.6) simply states that the energy per nucleon in nuclei is a minimum.

Secondly, the nuclei must be stable against  $\beta$ -decay. This is the statement that changing a proton (and electron) into a neutron must raise the energy, or in other words, that  $E_{\text{tot}}$  is minimized with respect to variations in  $Z$  at fixed  $A$ ,  $n_N$ ,  $V_N$  and  $n_n$ . Carrying out this minimization, using (2.2), yields the condition

$$\mu_e = - \frac{\partial}{\partial Z} (W_N + W_L)_{A, n_N, V_N, n_n} = - \frac{\partial}{\partial x} \left( \frac{W_N + W_L}{A} \right)_{A, n_N, V_N, n_n}, \quad (2.8)$$

where

$$\mu_e = \frac{\partial E_e}{\partial n_e} \quad (2.9)$$

is the electron chemical potential (including the rest mass).

The minimum energy (measured with respect to the neutron rest mass  $m_n$ ) required to add a neutron to a nucleus, i.e., the chemical potential of the neutrons in nuclei, is given by

$$\mu_n^{(N)} = \frac{\partial (W_N + W_L)}{\partial A} \Bigg|_{Z, n_N, V_N, n_n} - m_n c^2. \quad (2.10)$$

Similarly, the chemical potential of protons in nuclei (measured with respect to the proton rest mass  $m_p$ ) is given by the minimum energy required to add a proton to a nucleus at fixed neutron number  $A-Z$ :

$$\mu_p^{(N)} = \frac{\partial}{\partial Z} (W_N + W_L)_{A-Z, n_N, V_N, n_n} - m_p c^2. \quad (2.11)$$

In terms of the proton and neutron chemical potentials, the  $\beta$ -stability condition (2.8) reads

$$\mu_e - (m_n - m_p)c^2 = \mu_n^{(N)} - \mu_p^{(N)}. \quad (2.12)$$

This equation determines the electron chemical potential in terms of the nuclear parameters.

If  $\mu_n^{(N)}$  is negative, then there is no neutron gas outside the nuclei;  $\mu_n^{(N)}$  increases with increasing baryon density, and when it reaches zero <sup>†</sup>, neutrons begin to "drip" out of the nuclei. In order for the neutrons in the gas to be in equilibrium with those in nuclei, the neutron chemical potential,  $\mu_n^{(G)}$ , in the gas must equal that in the nuclei. This condition is derived by minimizing  $E_{\text{tot}}$  with respect to  $A$ , now at fixed  $V_N$ ,  $n_N$ ,  $Z$  and  $n_b$ , a variation corresponding to transferring a neutron from the gas to the nucleus, a process that should cost zero energy in equilibrium. At fixed  $n_b$ , we have

$$\frac{\partial n_n}{\partial A} = - \frac{n_N}{1 - V_N n_N}, \quad (2.13)$$

<sup>†</sup> Strictly speaking, the lowest energy of a free neutron state outside the nuclei differs slightly from zero due to the interaction of the neutron with the nuclei; this effect is very small however, since at the threshold for free neutrons, the nuclei occupy only about  $10^{-3}$  of the total volume of space.

so that

$$\begin{aligned} \frac{\partial E_{\text{tot}}}{\partial A} \Big|_{V_N, n_N, Z, n_b} &= 0 \\ &= n_N \left[ \frac{\partial}{\partial A} (W_N + W_L)_{V_N, n_N, Z, n_b} - \frac{\partial E_n}{\partial n_n} \right]. \end{aligned} \quad (2.14)$$

Using (2.10) and (2.13) we then find

$$\mu_n^{(G)} \equiv \left( \frac{\partial E_n}{\partial n_n} - m_n c^2 \right) + \frac{n_N}{1 - V_N n_N} \frac{\partial W_N}{\partial n_n} \Big|_{A, Z, V_N, n_N} = \mu_n^{(N)}. \quad (2.15)$$

We have used the fact that  $W_L$  is independent of  $n_n$ . The right side of (2.15) is the neutron chemical potential in the gas. The first term is the neutron chemical potential of the bulk neutron gas while the second term is the change in the nuclear surface energy caused by adding a neutron to the gas. In this term  $n_N W_N / (1 - V_N n_N)$  is the energy of nuclei per unit volume occupied by the outside neutron gas.

Lastly we write down the condition that equates the pressure of the outside neutron gas to that of the nucleus. This corresponds to minimizing  $E_{\text{tot}}$  with respect to  $V_N$  at fixed  $A$ ,  $Z$ ,  $n_N$  and  $n_n(1 - V_N n_N)$ , which is the total number of outside neutrons in a unit volume. We find then

$$P^{(N)} = P^{(G)}, \quad (2.16)$$

where

$$P^{(N)} = - \frac{\partial}{\partial V_N} (W_N + W_L) \Big|_{Z, A, n_n, n_N} \quad (2.17)$$

is the pressure on a nucleus, and

$$P^{(G)} = n_n \mu_n^{(G)} - (E_n - n_n m_n c^2) \quad (2.18)$$

is the outside neutron gas pressure. It may be verified that the total pressure

$$P = n_b^2 \frac{\partial}{\partial n_b} \left( \frac{E_{\text{tot}}}{n_b} \right) \quad (2.19)$$

is given by

$$P = P^{(G)} + P_e. \quad (2.20)$$

The charged particle contribution to the pressure is

$$P_e = P_e + P_L, \quad (2.21)$$

where

$$P_e = n_e^2 \frac{\partial}{\partial n_e} \left( \frac{E_e}{n_e} \right) \quad (2.22)$$

is the electron pressure and

$$P_L = n_N^2 \left( \frac{\partial W_L}{\partial n_N} \right)_{Z, A, V_N, n_n} \quad (2.23)$$

is the (negative) lattice pressure.

To summarize, the equilibrium conditions are given by (2.6), (2.8), (2.15) and (2.16). In order to make use of these conditions we must specify  $W_N$ ,  $W_L$ ,  $E_n$  and  $E_e$  explicitly. We turn now to this task.

### 3. Nuclear matter energy

The description of the nuclei that we shall study is that of compressible drops of nuclear matter. We write the energy  $W_N$  of a nucleus as a sum of a bulk energy, a surface energy and a Coulomb energy, in the spirit of the semi-empirical mass formula:

$$W_N(A, Z, V_N, n_n) = [(1-x)m_n c^2 + xm_p c^2 + W(k, x)]A + W_{\text{Coul}}(A, Z, V_N, n_n) + W_{\text{surf}}(A, Z, V_N, n_n). \quad (3.1)$$

Here  $W(k, x)$  is the energy per particle of bulk nuclear matter of density

$$n = \frac{k^3}{1.5\pi^2} \quad (3.2)$$

nucleons per unit volume, and  $x$  is the fractional concentration of protons. We consider now the determination of  $W(k, x)$ , and discuss in sects. 4 and 5 the surface and Coulomb energies.

In order to describe the matter within the nuclei and the outside neutron gas in a consistent manner, we use the same function  $W(k, x)$ , for  $x = 0$ , to describe the neutron gas, i.e.

$$\frac{E_n(n_n)}{n_n} = W(k_n, 0) + m_n c^2. \quad (3.3)$$

where

$$n_n = \frac{k_n^3}{1.5\pi^2} \quad (3.4)$$

(note that the neutron Fermi wave number equals  $2^{1/3}k_n$ ). In addition, the uniform neutron-proton fluid present at densities above that at which the nuclei dissolve is also described by the same function  $W(k, x)$ .

The standard methods of nuclear matter theory can be used to calculate  $W$ . In this theory one describes the nucleon-nucleon interaction by a two-body potential. The particular potential used in calculations described below was the Reid soft-core potential<sup>14)</sup>, which fits nucleon-nucleon scattering data below 300 MeV, as well as the properties of the deuteron, essentially within experimental error. Other potentials<sup>15)</sup>

do the same, but only a few of these also give good fits to nuclear matter, and those which do, do not differ greatly from the Reid soft-core potential.

One first calculates the correlation (wave function) of two interacting nucleons. For symmetric nuclear matter ( $x = \frac{1}{2}$ ) at nuclear densities this "pair approximation" gives a binding energy<sup>16)</sup> of 11 MeV per nucleon, compared with the empirical value  $\sim 16$  MeV. The remaining 5 MeV come from various corrections, the most important of which are the correlations between three<sup>17)</sup> and four<sup>18)</sup> interacting nucleons, and the three-nucleon forces arising from meson exchange<sup>19)</sup>. The methods of nuclear matter theory also give excellent results for the density distribution and energy levels of finite nuclei<sup>20)</sup>.

The energy of symmetric nuclear matter is of the form

$$W(k, \frac{1}{2}) = -w_0 + \frac{1}{2}K \left(1 - \frac{k}{k_0}\right)^2 \quad (3.5)$$

in the neighborhood of nuclear densities;  $w_0$  is  $\approx 16$  MeV, while  $k_0^3/1.5\pi^2$  is the saturation density,  $\approx 0.2$  nucleons per  $\text{fm}^3$ , or  $k_0 \approx 1.4 \text{ fm}^{-1}$ . The conventional compressibility parameter  $K$  has been calculated in the pair approximation<sup>16)</sup> to be  $\sim 135$  MeV.

For slightly unsymmetric ( $x \approx \frac{1}{2}$ ) nuclear matter one has

$$W(k, x) \approx W(k, \frac{1}{2}) + S(k)(1-2x)^2 \quad (3.6)$$

where the symmetry energy coefficient has been found by Siemens<sup>16)</sup> to have the approximate form

$$S(k) \approx 31 \left(\frac{k}{k_0}\right)^2 \text{ MeV} \quad (3.7)$$

(compared with the value of 28 MeV occurring in the Myers and Swiatecki semi-empirical mass formula). The approximate  $k^2$  dependence of the symmetry energy is due in part to the variation of the kinetic energy [see (3.15)], which near  $x = \frac{1}{2}$  behaves as  $(\hbar^2 k^2/6m_n)(1-2x)^2 \approx 14(k/k_0)^2(1-2x)^2$  MeV.

Nuclear matter theory has also been applied in calculating the properties of pure neutron matter<sup>8, 21-23)</sup>,  $x = 0$ . Here one expects the pair approximation alone to be quite good. The reason is that corrections to the nuclear matter energy coming from three- or more-body correlations, and especially the three-nucleon forces depend chiefly on tensor forces, which are important in triplet even states,  ${}^3\text{S}$  and  ${}^3\text{D}$ . However, triplet even states are forbidden for two neutrons (only  $T = 1$  states are possible) and hence these corrections are not important in pure neutron matter<sup>1</sup>.

<sup>1</sup> Ref.<sup>5)</sup> adopted the Németh and Sprung calculation "1a" of neutron matter, in which both isospin  $T = 0$  and  $T = 1$  interactions were increased by 22% to simulate the effects of three-body correlations and three-body forces. This correction makes their pair-approximation calculations for symmetric nuclear matter give 16 MeV binding energy. However, we now believe Németh and Sprung's calculation "1b", in which interactions in  $T = 1$  states were left unchanged while interactions in  $T = 0$  states were increased by 34%, to be the more reliable.

The most refined calculations for pure neutron matter are those of Siemens<sup>23</sup>); his results for the energy per particle can be fitted by the monotonically increasing function

$$W(k, 0) \approx 19.74k^2 - k^3 \frac{(40.4 - 1.088k^3)}{(1 + 2.545k)}, \quad (3.8)$$

(in MeV, and  $k$  in  $\text{fm}^{-1}$ ) for  $k \lesssim 1.5 \text{ fm}^{-1}$ . The first term in (3.8) is the kinetic energy,  $3\hbar^2(2^{1/2}k)^2/10m_n$ , of a free neutron gas, and is the dominant term at low densities.

Siemens' calculations do not include pairing correlations in the ground state. The effect of pairing on the energy has been estimated by Yang and Clark<sup>24</sup>), who find that while at very low neutron gas densities,  $k \sim 0.3$ , where the neutrons have little effect on the nuclei, the condensation energy can be as great as 25 % of the normal state energy, it is down to 10 % by  $k \sim 0.7$ , and falls rapidly with further increase in density. We shall not include these effects in  $W(k, x)$ .

The modification of  $W(k, x)$  for very small  $x$  involves the properties of a single proton in a pure neutron gas. Since the proton can be in relative  $T = 0$  states, three-body corrections are expected to play a role; these can be taken into account by the Németh-Sprung prescription<sup>†</sup> of increasing the  $T = 0$  interaction to get agreement in the pair approximation with the symmetric nuclear matter binding energy. The increase required in the Siemens pair-approximation calculation is  $\sim 30\%$ ; this is less than that required by Németh and Sprung since their pair-approximation calculation yields a lower binding energy than Siemens'. Increasing the  $T = 0$  interaction increases the effective attraction of protons to neutrons, which favors a larger percentage of protons in neutron matter of given density.

Siemens finds that the energy required to add a proton to a pure neutron gas, i.e., the proton chemical potential  $\mu_p^{(0)}$ , is fitted (for  $k \lesssim 1.5 \text{ fm}^{-1}$ ) by

$$\mu_p^{(0)} = -k^3 \frac{218 + 277k}{1 + 8.57k^2} \quad (3.9)$$

(in MeV and  $k$  in  $\text{fm}^{-1}$ );  $k^3/1.5\pi^2$  is the density of the neutron gas.

For small  $x$ , then,  $W$  has the form

$$W(k, x) = W(k, 0) + x(\mu_p^{(0)} - \mu_n^{(0)}), \quad (3.10)$$

where  $\mu_n^{(0)}$ , the chemical potential of pure neutron matter, is given by

$$\mu_n^{(0)}(k) = \frac{\partial E_n(n_n)}{\partial n_n} = W(k, 0) + \frac{1}{2}k \frac{\partial W(k, 0)}{\partial k}. \quad (3.11)$$

The next correction in powers of  $x$  comes from the proton kinetic energy and is given by

$$\frac{3\hbar^2[(2x)^{1/2}k]^2}{10m_p^*} x = 19.74k^2 x^{5/3} \frac{m_n}{m_p^*} (\text{MeV}); \quad (3.12)$$

<sup>†</sup> See preceding footnote.

$m_p^*(k)$  is the effective mass of a single proton in pure neutron matter. Not having calculations of  $m_p^*(k)$  we take it to be equal to  $m_n$ . One expects however that because of the strong proton-neutron attraction a single proton in a pure neutron gas will carry a considerable dressing cloud of neutrons with it, which will lead to a significant enhancement of the proton effective mass. This should be contrasted with symmetric nuclear matter where empirically  $m_p^*/m_n$  on the Fermi surface is close to unity (see e.g., ref.<sup>25</sup>), and where the average effective mass entering the calculation of the energy is  $m_p^*/m_n \approx 0.65$ .

In the absence of detailed calculations of  $W(k, x)$  for intermediate values of  $x$  between almost zero and nearly symmetric nuclear matter, we have, for use in calculations, interpolated  $W$  smoothly to fill in the gaps in our knowledge. In constructing the interpolation we have the following information about  $W$ :

(a) For symmetric nuclear matter in the neighborhood of saturation density  $W$  has the form:

$$W(k, \frac{1}{2}) = -w_0 + \frac{K}{2k_0^2} (k - k_0)^2. \quad (3.13)$$

(b) For small  $x$ , one has from eqs. (3.8)–(3.12):

$$W(k, x) = W(k, 0) + x(\mu_p^{(0)} - \mu_n^{(0)}) + \frac{3(2^{\frac{1}{3}}\hbar k)^2}{10m_n} x^{5/3}. \quad (3.14)$$

(c) At low  $k$ , the energy becomes just the free particle kinetic energy (ignoring free deuteron formation, which is not relevant here):

$$W_{kin}(k, x) = \frac{3(2^{\frac{1}{3}}\hbar k)^2}{10m_n} (x^{5/3} + (1-x)^{5/3}). \quad (3.15)$$

(d) The symmetry energy, that is, the correction to  $W$  as one moves away from  $x = \frac{1}{2}$ , is given for small

$$\alpha \equiv 1 - 2x \quad (3.16)$$

by

$$W_{symm} = W(k, x) - W(k, \frac{1}{2}) \approx \frac{sk^2}{k_0^2} \alpha^2. \quad (3.17)$$

We shall assume this  $k^2$  dependence to be valid in the range of  $k$  of interest.

First we do a polynomial interpolation, for  $x = \frac{1}{2}$ , between the  $k \approx k_0$  form (3.13) and the  $k \rightarrow 0$  form (3.15); written in a somewhat lengthy but transparent form we have:

$$\begin{aligned} W(k, \frac{1}{2}) = \frac{3\hbar^2 k^2}{10m_n} \left(1 - \frac{k}{k_0}\right)^3 - w_0 \left(\frac{k}{k_0}\right)^3 & \left[1 + \left(1 - \frac{k}{k_0}\right) \left(9 - 6 \frac{k}{k_0}\right)\right] \\ & + \frac{1}{2} K \left(1 - \frac{k}{k_0}\right)^2 \left(\frac{k}{k_0}\right)^3. \end{aligned} \quad (3.18)$$

To interpolate between  $x = 0$  and  $x = \frac{1}{2}$  we first subtract kinetic energy contributions from (3.14), (3.18) and the symmetry energy (3.17), and then construct the fit to the interaction energy as a polynomial in even powers of  $\alpha$  up to order  $\alpha^6$ . The resulting interpolation formula for  $W(k, x)$  is then:

$$\begin{aligned} W(k, x) = & \left[ W(k, \frac{1}{2}) - \frac{3\hbar^2 k^2}{10m_n} \right] (1 - 3\alpha^4 + 2\alpha^6) + \left[ s \left( \frac{k}{k_0} \right)^2 - \frac{\hbar^2 k^2}{6m_n} \right] \alpha^2 (1 - \alpha^2)^2 \\ & + \left[ W(k, 0) - \frac{3 \cdot 2^{\frac{1}{3}} \hbar^2 k^2}{10 m_n} \right] (3\alpha^4 - 2\alpha^6) + \left( \mu_p^{(0)} - \mu_n^{(0)} + 2^{\frac{1}{3}} \frac{\hbar^2 k^2}{2m_n} \right) \frac{1}{2} (\alpha^4 - \alpha^6) \\ & + W_{\text{kin}}(k, x). \end{aligned} \quad (3.19)$$

As  $x \rightarrow \frac{1}{2}$ , (3.19) agrees with (3.17) and (3.18), while as  $x \rightarrow 0$ , it agrees with (3.14). As  $k \rightarrow 0$ , (3.19) approaches

$$W_{\text{kin}} + \left[ 2 \left( \frac{k}{k_0} \right)^2 - \frac{\hbar^2 k^2}{6m_n} \right] \alpha^2 (1 - \alpha^2)^2; \quad (3.20)$$

the failure of the interaction part of the symmetry energy to drop out in this limit is due to the assumed  $k^2$  dependence being incorrect as  $k \rightarrow 0$ . At worst however, this

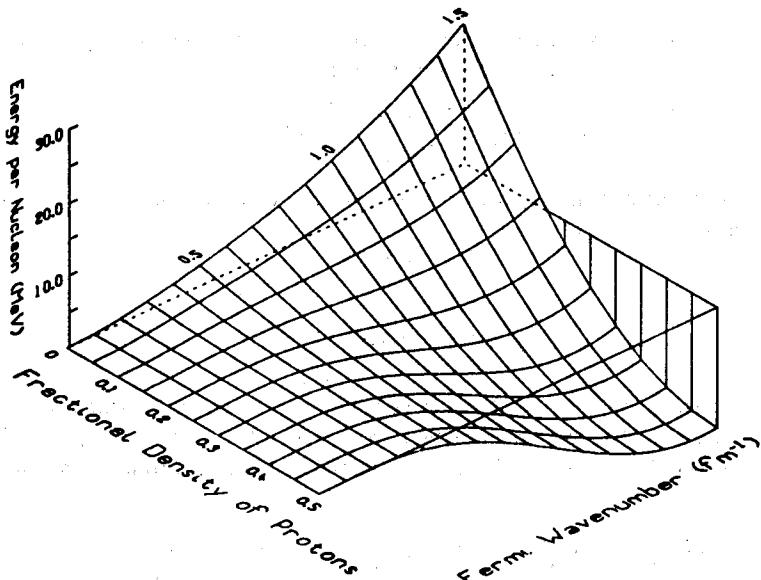


Fig. 1. Energy,  $W$ , per nucleon in bulk nuclear matter, as calculated from eq. (3.19), and plotted as a function of  $x$ , the fractional concentration of protons, and  $k$ , the mean Fermi wave number, related to the density of nucleons by  $n = k^3/1.5\pi^2$ . At  $x = 0$  and  $k = 1.5 \text{ fm}^{-1}$ ,  $W = 18.7 \text{ MeV}$ .

makes an  $\sim 15\%$  error in  $W$  in this limit. In any event, this is irrelevant, since we are never interested in  $W(k, x)$  at very low densities for finite  $x$ . Note that  $W(k, x)$  is symmetric about  $x = \frac{1}{2}$ .

The complete  $W(k, x)$  is shown in fig. 1. The parameters of nearly symmetric nuclear matter,  $w_0$ ,  $k_0$ ,  $K$  and  $s$  used here are:

$$w_0 = 16.5 \text{ MeV}, \quad k_0 = 1.43 \text{ fm}^{-1}, \quad K = 143 \text{ MeV}, \quad s = 33.0 \text{ MeV}. \quad (3.21)$$

These were chosen empirically by fitting our compressible liquid-drop nucleus model to the binding energies and radii of real stable nuclei<sup>26</sup>; the parameters (3.21) are in fact quite close to the values calculated by nuclear matter theory<sup>16-19</sup>. The fact that  $w_0$  and  $s$  differ somewhat from the values  $w_0 = 15.7$  MeV and  $s = 1.79 w_0 = 28.1$  MeV of Myers and Swiatecki's mass formula<sup>7</sup>) is primarily due to our fixing the Coulomb energy from measured nuclear sizes, rather than treating it as an empirical quantity to be determined from binding energies. The effective value of our symmetry energy coefficient is  $(k/k_0)^2 s$ , which for  $k \approx 1.35 \text{ fm}^{-1}$  equals 29.3 MeV, a value close to that of Myers and Swiatecki.

The possibility of having nuclei immersed in a neutron fluid may be viewed as the coexistence of nuclear matter at two separate densities and proton concentrations. While the finer details of the coexistence densities and proton concentration depend on finite-size effects, namely Coulomb and surface energies, these effects, as we shall see, become small as the density of the outside neutron gas approaches the density of matter inside the nuclei. The major features of the coexistence between nuclear matter and a pure neutron gas are determined primarily by the properties of bulk matter, as described by  $W(k, x)$ , neglecting Coulomb forces.

In order for a pure neutron gas to be in equilibrium with nuclear matter, the pressures, as well as the neutron chemical potentials in the two phases, must be equal. In fig. 2 we have plotted the neutron and proton chemical potentials of the bulk matter, given by

$$\begin{aligned} \mu_n &= W + \frac{k}{3} \frac{\partial W}{\partial k} - x \frac{\partial W}{\partial x}, \\ \mu_p &= \mu_n + \frac{\partial W}{\partial x}, \end{aligned} \quad (3.22)$$

as a function of  $x$ , the fractional concentration of protons, for a number of fixed pressures:

$$P = \frac{k^3}{1.5\pi^2} \left( \frac{1}{2} k \frac{\partial W}{\partial k} \right). \quad (3.23)$$

The upper curves are the neutron chemical potentials while the lower are the proton chemical potentials. The  $\mu_p$  and  $\mu_n$  curves meet, for each pressure, at  $x = \frac{1}{2}$ .

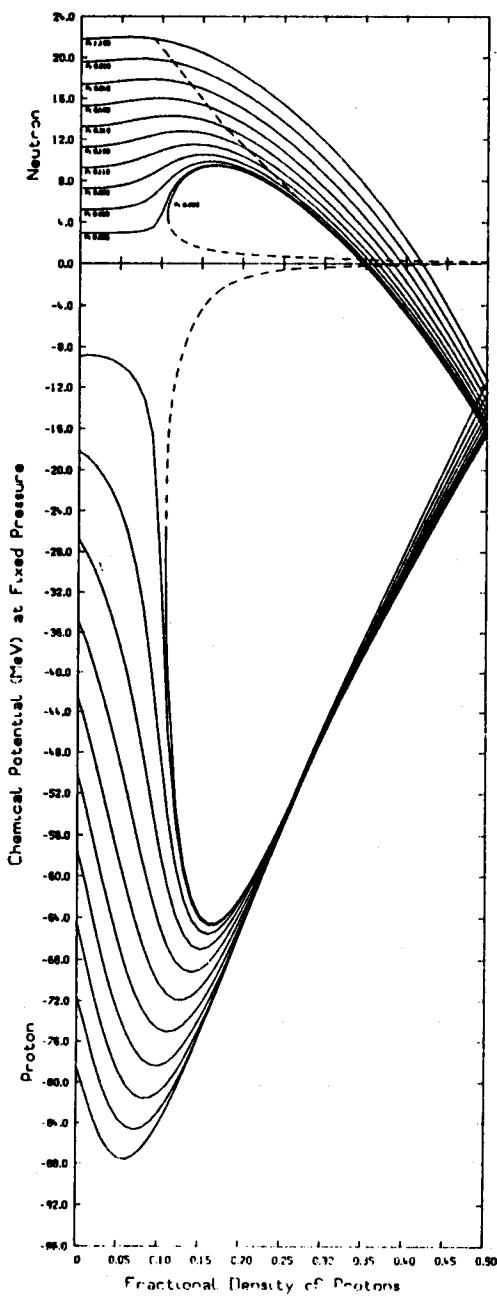


Fig. 2. The neutron and proton chemical potentials for bulk nuclear matter, plotted for given pressures  $P$  as a function of  $x$ , the fractional density of protons. The pressures, constant along each curve, are measured in MeV/fm $^3$ . The neutron chemical potential ( $\mu_n$ ) curves begin for  $x = 0$ , at positive values, while the proton chemical potentials ( $\mu_p$ ) begin at negative values at  $x = 0$ . Note that  $\mu_p(P, x = 0)$  decreases with increasing pressure. The dashed line intersecting the  $\mu_n$  curves is the coexistence curve; for a given value of  $\mu_n$ , this curve tells the proton concentration of bulk matter that has the same pressure as, and hence can coexist with, a pure neutron gas at the given  $\mu_n$ . The  $P = 0$  curve, starting at saturated symmetric nuclear matter,  $x = \frac{1}{2}$ ,  $\mu_p = \mu_n = -16.5$  MeV, never reaches concentrations lower than  $x \approx 0.11$ , but instead it doubles back; matter corresponding to the dashed region of the  $P = 0$  curve has negative compressibility and hence is unstable. It can be seen that for any point on the coexistence curve, the value of  $\mu_p(P, x)$  is always greater than  $\mu_p(P, 0)$ , indicating that proton drip does not occur for bulk matter. Also it can be seen that it is impossible to have coexistence, that is, equal  $\mu_n$  and  $P$  between two phases each with finite proton concentration.

To construct the coexistence curve we first pick a pressure for the pure neutron gas. This fixes the value of  $\mu_n$  and hence the density of the pure neutron gas. The nuclear matter that can coexist with the neutron gas obeys  $\mu_n(x, P) = \mu_n(0, P)$ ; its value of  $x(P)$  can be read from the graph. The dashed line is the coexistence curve.

The concentration of protons in the coexisting nuclear matter falls steadily with increasing  $\mu_n$ , while it may be shown that the density, or  $k$ , falls slightly as  $\mu_n$  increases, goes through a minimum, and then rises slightly. There appears to be no equilibrium possible in bulk for  $\mu_n \gtrsim 30$  MeV, which corresponds to a limiting density  $\sim 4 \times 10^{14}$  g/cm<sup>3</sup>, a little greater than symmetric nuclear matter density. One can also see that along the coexistence curve the proton chemical potential in the nuclear matter is always less than that in the pure neutron gas, i.e.,  $\mu_p(x, P) < \mu_p(0, P)$  when  $\mu_n(x, P) = \mu_n(0, P)$ . Thus there is no tendency in bulk matter for "proton drip".

#### 4. Nuclear surface energy

The energy density in the interior of nuclei can be described by the calculations for uniform nuclear matter discussed in sect. 3. This volume energy,  $W(k, x)$  per nucleon, includes through its  $x$ -dependence the symmetry energy, and through its density dependence, the effect of a finite neutron gas pressure outside the nuclei. The Coulomb energy of the nuclei, including the important Coulomb interaction between nuclei, is straightforward to evaluate, and will be considered in the next section. We look now at the nuclear surface energy.

As the density of the matter, and hence the density of neutrons outside the nuclei grows, the nuclear surface energy decreases. This is because the matter inside the nuclei becomes more and more neutron rich, and at the same time the density difference between the matter inside and outside the nuclei becomes small. Were the matter inside and outside the nuclei the same there would, of course, be no surface energy. We shall attempt now to construct an approximate formula for the nuclear surface energy (as a function of the matter densities  $n_i$  and  $n_o$  inside and outside the nuclei, and the  $Z$  and  $A$  of the nuclei) that accounts for this lowering of the surface energy.

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**Neutron Star Models with Realistic High-Density  
Equations of State**  
(with R. C. Malone and M. B. Johnson)  
*Astrophys. J.* **199**, 741–748 (1975)

Using equations of state derived previously by Bethe and Johnson, the density distribution in neutron stars is derived. The maximum mass of a neutron star is found to lie between  $1.65$  and  $1.85 M_{\odot}$ , only slightly greater than Chandrasekhar's limit for white dwarfs,  $1.45 M_{\odot}$ . In 1994, it was suggested that at high density,  $K^-$  mesons form a condensate in nuclear matter: assuming this, the maximum mass may be as low as  $1.50 M_{\odot}$  which fits well with the statistics of observed neutron stars.

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## NEUTRON STAR MODELS WITH REALISTIC HIGH-DENSITY EQUATIONS OF STATE

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### ABSTRACT

We calculate neutron star models using four realistic high-density models of the equation of state. We conclude that the maximum mass of a neutron star is unlikely to exceed  $2 M_{\odot}$ . All of the realistic models are consistent with current estimates of the moment of inertia of the Crab pulsar.

*Subject headings:* dense matter — equation of state — neutron stars — pulsars

#### I. ASTROPHYSICAL CONSIDERATIONS

The discovery of pulsars and recent investigations of strong galactic X-ray sources have given a great impetus to the study of neutron star properties. It is now generally accepted that pulsars are rotating neutron stars with strong magnetic fields (Gold 1968), although the pulsar emission mechanism is not fully understood. The principal reservoir of energy in a pulsar is customarily assumed to be the kinetic energy of rotation of the neutron star. In the case of the Crab Nebula and its pulsar, the rate of conversion of this energy must suffice to supply the observed energy losses to charged particles, nebular radiation, and accelerated nebular expansion (if it occurs). The rate of decrease of the rotational energy is

$$\dot{E} = I\Omega\dot{\Omega}, \quad (1.1)$$

where  $I$  is the moment of inertia of the neutron star, and  $\Omega$  and  $\dot{\Omega}$  are the angular frequency of rotation and its time derivative. Ruderman (1972) has compared equation (1.1) using  $\Omega$  and  $\dot{\Omega}$  for the Crab pulsar with observation-based estimates of the apparent accelerated expansion of the Crab Nebula (Trimble and Rees 1970); the upper limit of the observed energy loss is somewhat in excess of that attainable from equation (1.1) even with the maximum  $I$  calculated by Baym, Pethick, and Sutherland (1971) using a high-density hyperonic equation of state of Pandharipande (1971). One purpose of the present paper is to investigate the latitude in the maximum value of  $I$  permitted by the uncertainties in the equation of state at supranuclear densities.

Similar considerations apply to the maximum mass of a neutron star. A number of X-ray sources located in binary systems have been discovered recently (Dolan 1971; Schreier *et al.* 1972; Tananbaum *et al.* 1972;

Ulmer *et al.* 1972). Observations of the massive companions in Cygnus X-1 (Webster and Murdin 1972; Bolton 1972) and Vela X-1 (Vidal, Wickramasinghe, and Peterson 1973; Wickramasinghe *et al.* 1974) have suggested that the minimum masses of the compact companions in these two sources may exceed  $3 M_{\odot}$ , and improved estimates of the distance to Cygnus X-1 (Margon *et al.* 1973; Bregman *et al.* 1973) raise that value to  $6 M_{\odot}$ . Previous calculations of neutron star models with the high-density equations of state then available have indicated that the maximum mass of a stable neutron star lies in the range  $1.5-2 M_{\odot}$  (Börner and Sato 1971; Clark *et al.* 1971; Baym *et al.* 1971). Because this mass is below that estimated for the masses of the compact companions, it is particularly interesting to see how far the maximum mass of a neutron star can be pushed, subject to the constraints of the present-day theory of hyperonic matter.

We consider four equations of state based on different assumptions concerning the interactions of nucleons, hyperons, and nucleon resonances. These assumptions are consistent with known experimental information and represent, in our opinion, reasonable bounds upon the state of hyperonic matter, at least insofar as the relation of pressure to energy density is concerned. The various assumptions and the resultant states of hyperonic matter are presented in § II; for a more comprehensive discussion of hyperonic matter, see Bethe and Johnson (1974).

A recent alternative equation of state has been derived by Pandharipande and Smith (1974) based on the Green-Haapakoski (1974) theory of the nuclear interaction. This theory is different from the theory of Bethe and Johnson (1974), but does not lead to substantially different star properties (see § IV).

While we follow the customary practice of assuming that Einstein's theory of general relativity is the correct theory of gravitation, experiment has yet to rule out all classes of gravitational theories which differ significantly from Einstein's theory (Thorne and Will

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1971; Will and Nordtvedt 1972; Thorne, Will, and Ni 1971). Some recent work by Wagoner and Malone (1974) which applied other theories of gravitation to neutron star models (by way of the Parametrized Post-Newtonian [PPN] formalism) indicates that other gravitational theories might give rise to significantly larger maximum masses, for the same equation of state, than those obtained from general relativity. By varying a parameter (of the PPN theory) which is as yet poorly determined experimentally, it was found (Wagoner and Malone 1974) that in the range where post-Newtonian theory is applicable, models could be obtained with gravitational masses 2 to 3 times larger than the general-relativistic models of the same central density. However, the post-Newtonian theory could not be applied near the maximum stable mass. Hopefully, future experiments will greatly reduce the uncertainty in this parameter.

Sections III and IV discuss the method of calculation of the neutron star models and the results, respectively.

## II. EQUATION OF STATE

To estimate the uncertainties in neutron star properties due to our imperfect knowledge of the equation of state, we have done stellar structure calculations using four models obtained from the work of Bethe and Johnson (1974), which apply in the density range  $n_B \geq n_0$  ( $n_0 \equiv$  normal nuclear matter density =  $0.16 \text{ fm}^{-3}$ ). The primary reason for the uncertainties is that densities  $n_B > n_0$  are not available for study in terrestrial laboratories.

For densities  $n_B < n_0$  the equation of state is known with much greater accuracy. It divides naturally into the following three ranges (the references cited refer to the work from which we take the equation of state):

1. For<sup>1</sup>  $\rho = m_n n_B < 10^7 \text{ g cm}^{-3}$ , the state of minimum energy is <sup>56</sup>Fe, arranged in a lattice to minimize the Coulomb energy (Feynman, Metropolis, and Teller 1949). This phase is confined to the outermost layer of the neutron star and is of no consequence to its overall structure.

2. For  $10^7 < \rho < 4 \times 10^{11} \text{ g cm}^{-3}$ , equilibrium matter still consists of nuclei in a lattice, but the neutron number is larger than for isolated nuclei (Baym *et al.* 1971).

3. At a density  $\rho$  of about  $4 \times 10^{11} \text{ g cm}^{-3}$  the nuclei have become so neutron-rich that neutrons begin to "drip" out of the nuclei. From the density  $4 \times 10^{11}$  to  $2.4 \times 10^{14} \text{ g cm}^{-3}$ , matter is characterized by a neutron gas (superfluid) coexisting with large, neutron-rich nuclei in a lattice (Baym, Bethe, and Pethick 1971 [referred to hereafter as BBP]; Ravenhall, Bennett, and Pethick 1972). At this point the nuclei disappear, giving way to uniform neutron liquid with a small percentage of protons and electrons dissolved in it.

Except for low-mass stars, the equation of state in density ranges (2) and (3) are relatively unimportant

<sup>1</sup> Here  $m_n$  is the neutron mass. In these units nuclear matter density  $\rho_0 = 2.4 \times 10^{14} \text{ g cm}^{-3}$ .

for the overall structure; the most important density range is  $\rho > \rho_0$ , which we discuss next.

For densities  $\rho > \rho_0$ , calculations of the equations of state rely heavily on many-body theory. For our calculations we take models obtained by Bethe and Johnson (1974) from the variational theory of Pandharipande (1971) under the assumption that matter is liquid at these densities. The different models are based on underlying interactions which are consistent with experiments (for criteria used, see below). These potentials constitute an improvement over those currently used in nuclear physics.

The differences between the models are the underlying interaction. Bethe and Johnson took potentials which act differently depending on the angular momentum of the interacting pairs of particles. The coefficients of the potential (the potentials are sums of Yukawa forms) were fit to the data as outlined in the criteria (a)-(g).

a) The potential should have a repulsive core in all states.

b) The core strength should satisfy the inequality

$$V_c(^1P) \geq V_c(^3P) \geq V_c(^3S) \geq V_c(^1S).$$

c) The nucleon-nucleon interaction must give the correct experimental phase shifts for energies up to 350 MeV, and the correct binding energy and quadrupole moment of the deuteron, like Reid's (1968).

d) The nucleon-nucleon interaction must saturate nuclear matter at a reasonable density and energy.

e) Hyperonic interactions must be consistent with the (meager) experimental measurements, in particular measurements of hypernuclei. These indicate that the hyperon-nucleon attraction is less than the nucleon-nucleon, but not by much.

f) It is desirable, but not necessary, that the repulsive core have the same range in all states.

g) It is desirable that the short range repulsion have a range corresponding to the exchange of  $\omega$ -mesons.

All of the equations of state are qualitatively similar. At densities  $\rho > \rho_0$  the composition is mostly neutrons with few protons and electrons. With increasing density the concentrations of these charged particles increase. At the higher densities the hyperons  $\Sigma$ ,  $\Lambda$ , and  $\Delta_{33}$  were constituents of matter. The  $\Sigma^-$  was the first to appear, and the threshold was  $n_B \approx 0.5 \text{ fm}^{-3}$ . However, the hyperons had very little effect on the equation of state.

All four equations of state are presented numerically in Table 1, with analytic expressions which may be used at the higher densities. Of the four, model I H is the least sophisticated. It was assumed that all baryons interact in the same way, except for like nucleons, which were taken to have extra attraction in states of relative orbital angular momentum  $l = 0$ . The equality in criterion (b) was satisfied, with the strength and range of the repulsive term taken from the Reid (1968)  $^1S_0$  potential. The range of the repulsion is short in this model and its strength large, when compared with the values preferred by high-energy measurements of the  $\omega$ -meson. This potential is an

TABLE I  
REALISTIC HIGH-DENSITY\* AND CAUSALITY-LIMIT EQUATIONS OF STATE

$n_B(\text{fm}^{-3})$	$\frac{\epsilon}{n_B} - m_nc^2 \text{ (MeV)}$					$\epsilon(10^{35} \text{ ergs cm}^{-3})$					$P(10^{33} \text{ dyn cm}^{-2})$				
	I	III	V N	V H	CLM	I	III	V N	V H	CLM	I	III	V N	V H	CLM
0.1.....	16.8	14.1	12.6	12.6		1.52	1.53	1.53	1.53		1.74	1.49	1.19	1.19	
0.15.....	22.8	18.6	16.6	16.6		2.29	2.31	2.29	2.29		4.55	3.39	2.93	2.93	
0.2.....	29.7	23.5	21.2	21.2		3.08	3.09	3.07	3.07		9.36	6.49	6.00	6.00	
0.25.....	37.5	29.0	26.0	26.0		3.89	3.88	3.87	3.87		16.5	11.1	10.9	10.9	
0.3.....	46.0	34.6	32.2	32.2	32.2	4.71	4.68	4.68	4.68	4.68	26.1	17.3	18.3	18.3	18.3
0.4.....	65.3	47.5	46.9	46.9	83.8	6.43	6.33	6.33	6.33	6.57	55.3	36.5	40.9	40.9	207
0.5.....	88.4	63.3	64.4	64.4	183	8.23	8.04	8.04	8.04	9.00	99.6	68.0	76.1	76.1	450
0.6.....	115	82.0	83.7	83.7	301	10.1	9.82	9.84	9.84	12.0	162	114	126	126	750
0.7.....	144	104	109	109	436	12.2	11.7	11.8	11.8	15.5	241	180	199	199	1100
0.8.....	178	129	134	134	579	14.3	13.7	13.8	13.8	19.5	337	266	285	285	1500
0.9.....	211	156	160	160	694	16.6	15.8	15.8	15.8	24.1	450	334	371	371	1960
1.0.....	247	185	190	189	847	19.0	18.1	18.1	18.3	29.3	587	485	492	492	2480
1.1.....	284	221	224	215	1036	21.6	20.5	20.5	20.6	34.9	742	604	623	502	3040
1.25.....	344	270	274	254	1273	25.7	24.2	24.3	24.2	44.4	1020	837	858	676	3990
1.4.....	406	322	327	295	1513	30.2	28.3	28.4	28.1	55.1	1350	1120	1140	881	5060
1.5.....	450	358	360	324	1674	33.4	31.2	31.3	30.8	63.0	1610	1330	1340	1030	5850
1.7.....	542	435	442	383	1999	40.3	37.4	37.7	36.6	80.3	2180	1830	1855	1380	7580
2.0.....	689	559	560	475	2491	52.2	48.0	48.1	46.2	110	3270	2780	2758	2020	10550
2.5.....	959	790	788	639	3317	76.0	69.3	69.2	64.8	171	5690	4910	4831	3400	16650
3.0.....	1260	1050	1040	814	4147	106	95.5	95.3	86.6	245	8940	7810	7623	5200	24050

\* Bethe and Johnson 1974.

Model I H:

$$\left. \begin{aligned} \epsilon &= n_B(15.05 + 3.96n_B^{1.48})10^{35} \text{ ergs cm}^{-3} \\ P &= 586n_B^{2.48}10^{33} \text{ dyn cm}^{-2} \end{aligned} \right\} n_B \geq 0.8 \text{ fm}^{-3}$$

Model III H:

$$\left. \begin{aligned} \epsilon &= n_B(15.05 + 3.06n_B^{1.65})10^{35} \text{ ergs cm}^{-3} \\ P &= 474n_B^{2.65}10^{33} \text{ dyn cm}^{-2} \end{aligned} \right\} n_B \geq 1.0 \text{ fm}^{-3}$$

Model V N:

$$\left. \begin{aligned} \epsilon &= n_B(14.89 + 3.25n_B^{1.508})10^{35} \text{ ergs cm}^{-3} \\ P &= 490n_B^{2.508}10^{33} \text{ dyn cm}^{-2} \end{aligned} \right\} n_B \geq 0.7 \text{ fm}^{-3}$$

Model V H:

$$\left. \begin{aligned} \epsilon &= n_B(15.05 + 3.03n_B^{1.83})10^{35} \text{ ergs cm}^{-3} \\ P &= 403n_B^{2.83}10^{33} \text{ dyn cm}^{-2} \end{aligned} \right\} n_B \geq 1.0 \text{ fm}^{-3}$$

improvement over the Reid (1968) potential, as is the case for the other models. The best previous calculations of the equation of state of hyperonic matter were based on the Reid potential (Pandharipande 1971). The improvements make the equation of state stiffer.

Model III H differs from model I H because it is based on a more realistic choice of potential for neutrons and protons in states of relative orbital angular momentum  $l = 0$  and 1; however, the strength and range of the central part of the repulsive term is the same as for model I H. Comparison with model I H shows that these improvements make the pressure less for a given baryon density  $n_B$ .

Interaction model V differs from the preceding in that the inequality (b) was satisfied. In addition, the parameters for the repulsive core were closer to those which are preferred by high-energy measurements of the  $\omega$ -meson. However, the strength of the repulsion is still too large. Smaller strengths for this term resulted in worse fits to the experimental phase shifts. We choose the two cases, models V H and V N, corresponding to this interaction model. The former allows hyperons, while the latter assumes pure neutron matter. Model V H is noticeably softer at the higher densities than V N because of the softening effect of hyperons. Model V H is the softest model considered. Model V N is numerically very similar to model III H. We have matched these equations of state to the BBP equation of state gradually over the density range  $n_B = 0.118 \text{ fm}^{-3}$  to  $n_B = 0.20 \text{ fm}^{-3}$ .

The four high-density equations of state discussed are quite similar despite the variety of assumptions concerning particle interactions at short distances made in deriving them. However there remains some uncertainty concerning such interactions, and therefore a rigorous upper limit to the equation of state is of interest. Causality requires that the velocity of sound in matter,  $v_s$ , not exceed the velocity of light:

$$\left(\frac{v_s}{c}\right)^2 = \left(\frac{\partial P}{\partial \epsilon}\right)_S \leq 1, \quad (2.1)$$

where  $P$  is the pressure,  $\epsilon$  the total energy density, and the derivative is taken at constant entropy  $S$  (Thorne 1966). This restriction has been discussed for both quantum and classical systems in a series of papers by Bludman and Ruderman (1968, 1970) and Ruderman (1968).

If we assume that the equation of state is well known for densities below some value  $\rho^*$ , then the stiffest (greatest  $P$  for a given  $\rho$ ) possible equation of state above  $\rho^*$  is

$$P = P^* + (\epsilon - \epsilon^*), \quad (2.2)$$

where  $P^* = P(\rho^*)$  and  $\epsilon^* = \epsilon(\rho^*)$ . The baryon number density is determined by the thermodynamic relation

$$P = n_B^2 d(\epsilon/n_B)/dn_B, \quad (2.3)$$

which, with equation (2.2), can be integrated to yield

$$n_B = n_B^* [1 + 2(\epsilon - \epsilon^*)/(\epsilon^* + P^*)]^{1/2}, \quad (2.4)$$

where  $\rho^* \equiv n_B^* m_n$ . Rhoades and Ruffini (1974) have shown that relative to any other possible equations of state, equation (2.2) maximizes the mass of a neutron star model.

For comparison with the hyperon matter equations of state, "causality limit" neutron star models (CLM) were computed using equation (2.2), which was matched to model V at a density  $n_B^* = 0.3 \text{ fm}^{-3}$ .

### III. CALCULATIONS

In the present work, the theory of gravitation was taken to be Einstein's theory of general relativity. We define the metric as

$$ds^2 = e^{2\Phi} c^2 dt^2 - (1 - 2Gm/rc^2)^{-1} dr^2 - r^2(d\theta^2 + \sin^2 \theta d\phi^2), \quad (3.1)$$

where  $r$  is the proper radius,  $m(r)$  is the gravitational mass contained within  $r$ ,  $G$  is the Newtonian constant of gravitation, and  $c$  is the speed of light. The potential  $\Phi(r)$  relates the element of proper time  $d\tau = e^\Phi dt$  to the element of time measured at  $r = \infty$ ,  $dt$ ; hence  $\Phi(\infty) = 0$ . The equation of hydrostatic equilibrium is (Thorne 1966)

$$\frac{dP}{dr} = -\frac{G}{r^2 c^2} \frac{(\epsilon + P)(m + 4\pi r^3 P/c^2)}{1 - 2Gm/rc^2}, \quad (3.2)$$

where  $P$  is the pressure and  $\epsilon$  is the total mass-energy density. In addition,

$$\frac{dm}{dr} = 4\pi r^2 \epsilon / c^2, \quad (3.3)$$

$$\frac{d\Phi}{dr} = \frac{G}{r^2 c^2} \frac{m + 4\pi r^3 P/c^2}{1 - 2Gm/rc^2}. \quad (3.4)$$

The surface of the star,  $r = R$ , is defined by  $P(R) = 0$ , and the total gravitational mass is  $M_g = m(R)$ . Because  $P = 0$  and  $m = M_g$  for  $r > R$ , equation (3.4) can be integrated to give

$$\exp[\Phi(r)] = (1 - 2GM_g/rc^2)^{1/2} \quad (r \geq R). \quad (3.5)$$

We also define a conserved mass  $M_c = m_n B(R)$ , where  $m_n$  is the neutron rest mass and the number of baryons contained within radius  $r$ ,  $B(r)$ , is given by

$$\frac{dB}{dr} = 4\pi r^2 n_B(r) (1 - 2Gm/rc^2)^{-1/2}, \quad (3.6)$$

where  $n_B(r)$  is the baryon number density. The binding mass  $M_{\text{bind}}$  is defined as  $M_c - M_g$ .

Finally, we wish to calculate the moment of inertia,  $I$ . For a slowly rotating star,  $I$  can be determined from the structure of the nonrotating model (Thorne 1969). Let  $\Omega$  be the angular velocity of uniform rotation measured at infinity, and let  $\bar{\omega}(r)$  be the angular velocity of the fluid relative to particles with zero angular momentum. Due to the dragging of inertial frames,  $\bar{\omega}(r) \neq \Omega$ . If

$$\xi(r) = \exp[-\Phi(r)] (1 - 2Gm/rc^2)^{1/2},$$

$\bar{\omega}(r)$  satisfies the equation

$$\frac{1}{r^4} \frac{d}{dr} \left( r^4 \xi \frac{d\bar{\omega}}{dr} \right) + \frac{4}{r} \frac{d\xi}{dr} \bar{\omega} = 0 \quad (3.7)$$

and the boundary conditions  $(d\bar{\omega}/dr)_{r=0} = 0$  and  $\bar{\omega}(\infty) = \Omega$ . Outside the star  $\bar{\omega}(r) = \Omega - 2GJ/r^3c^2$ , so that

$$J = \frac{c^2}{6G} R^4 \left( \frac{d\bar{\omega}}{dr} \right)_{r=R}, \quad (3.8)$$

where  $J$  is the angular momentum of the star. Equation (3.5) shows that  $\xi(R) = 1$ ; however, because equation (3.7) is linear in  $\xi$ , for purpose of integration,  $\Phi(r)$  need only be defined to within an additive constant. Likewise  $\bar{\omega}(0)$  can be taken as any nonzero constant, since  $\bar{\omega}(r)$ ,  $\Omega$ , and  $J$  can all be scaled after the integration. This scaling does not affect  $I$ , which is defined as

$$I = J/\Omega. \quad (3.9)$$

The integration of equation (3.7) is conveniently carried out in terms of the auxiliary variable  $u = r^4(d\bar{\omega}/dr)$  which gives two coupled first-order equations:

$$\frac{du}{dr} + \frac{d(\ln \xi)}{dr} (u + 4r^3\bar{\omega}) = 0, \quad (3.10)$$

$$\frac{d\bar{\omega}}{dr} = \frac{u}{r^4}.$$

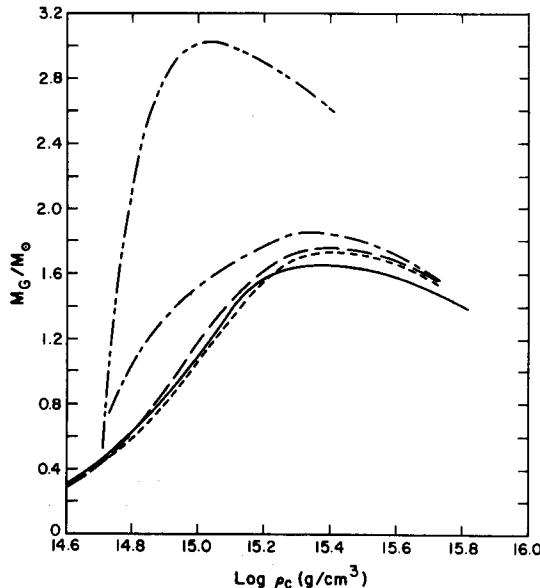


FIG. 1.—Gravitational mass  $M_G$  versus central baryon density  $\rho_c = m_n n_{B,c}$ , where  $m_n$  is the neutron rest mass and  $n_B$  is the baryon number density, for model I H (----), model III H (-----), model V H (—), model V N (— —), and the causality limit model (— · —).

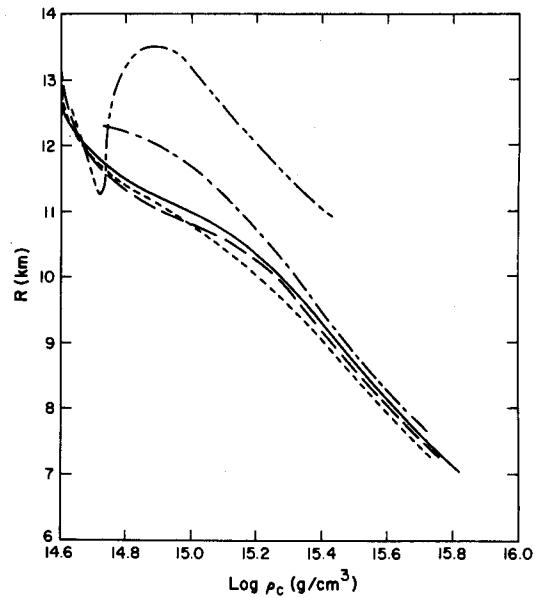


FIG. 2.—Neutron star radius  $R$  versus central baryon density  $\rho_c$ . See Fig. 1 for curve designations.

Equations (3.2)–(3.4), (3.6), and (3.10) can be numerically integrated outward from  $r = 0$  when an equation of state  $P = P(e)$  is specified. The computer code which does the integration was modeled after that described by Baym *et al.* (1971); the interested reader should consult that paper for further details.

#### IV. RESULTS AND DISCUSSION

The results of the calculation are shown in Figures 1–5 and in Table 2. The baryon density  $\rho = m_n n_B$  has been used consistently to facilitate comparisons with different equations of state. Stars having central densities  $\rho_c$  less than the matching density are identical in all models we have considered, and the results are therefore not shown. For properties of these stars, see Baym *et al.* (1971). For  $\rho_c$  greater than the matching density, star models show a spread in properties which reflect the uncertainties in the nuclear theory at high density; this sensitivity is of primary interest in our work. It is clear from Figures 1–4 that the range of assumptions made in deriving the various realistic high-density equations of state did not have a significant effect on the neutron star properties, as all of the maximum masses lie in the range  $1.65$ – $1.85 M_\odot$ . Table 2 shows the extremal properties of the stars; the variations in these quantities for the different equations of state are only about 10 percent, excluding the CLM.

Trimble and Rees (1970) have estimated the power required to drive the nebular expansion of the Crab Nebula at 2 to  $4 \times 10^{38}$  ergs s $^{-1}$ . With  $\Omega = 190$  rad s $^{-1}$  and  $\Omega = -2.44 \times 10^{-9}$  rad s $^{-2}$  (Ruderman 1972), a moment of inertia of  $8.6 \times 10^{44}$  g cm $^2$  is required if the larger value is to be supplied entirely by the conversion of rotational kinetic energy. Figure 3

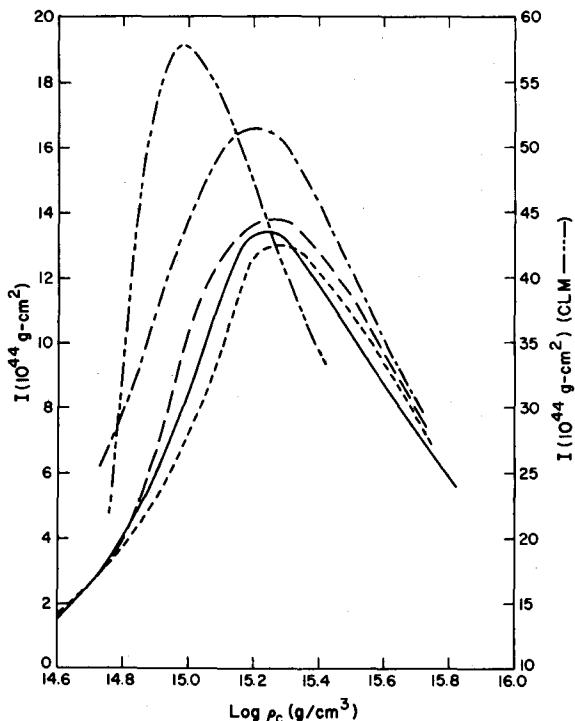


FIG. 3.—Moment of inertia  $I$  versus central baryon density  $\rho_c$ . See Fig. 1 for curve designations.

indicates that all of these equations of state can satisfy that requirement for masses in excess of  $1 M_\odot$ . Figure 5 shows the density versus radius of a typical star; the slight break at  $4 \times 10^{11} \text{ g cm}^{-3}$  reflects the softening of the BBP equation of state at the onset of neutron drip.

The results for the causality limit equation of state (CLES) are also presented in the Figures 1-4 and Table 2. Qualitatively, the much stiffer causality limit equation of state leads to higher values of  $M_G$ ,  $M_C$  (hence total baryon number),  $R$ , and  $I$ , and lower values of  $\rho_c$  than for the realistic equations of state. The CLES was joined onto the model V equation of state at a density  $\rho = 5 \times 10^{14} \text{ g cm}^{-3} \equiv \rho^*$ . This is

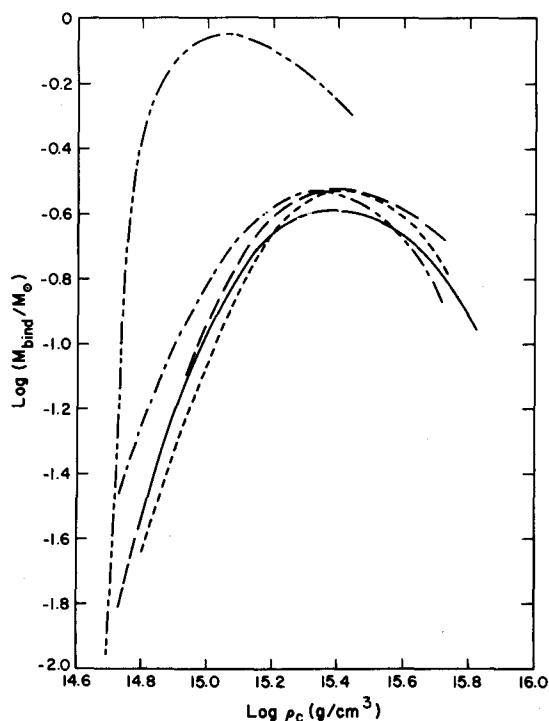


FIG. 4.—Binding mass  $M_{\text{bind}} = M_C - M_G$  versus central baryon density  $\rho_c$ . See Fig. 1 for curve designations.

slightly in excess of the highest density for which the equation of state of neutron star matter is known with much confidence. It should be pointed out that the maximum stable mass of a neutron star calculated with the CLES is a very sensitive function of the matching density  $\rho^*$ . Nauenberg and Chapline (1973) have shown in an approximate analytic theory that  $M_{G,\max} \propto (\epsilon^* - P^*)^{-1/2}$ . Since  $P^* \ll \epsilon^* \approx \rho^* c^2$  near nuclear density, it is important to use the highest acceptable values of  $\rho^*$  in order to obtain the most stringent upper bound on  $M_{G,\max}$ . For example, with  $\rho^* = 5 \times 10^{14} \text{ g cm}^{-3}$ ,  $M_{G,\max} = 3.0 M_\odot$ ; but with  $\rho^* = 2 \times 10^{14} \text{ g cm}^{-3}$ ,  $M_{G,\max} = 4.8 M_\odot$ . The same considerations apply to the maximum moment of inertia. On the basis of the calculations with the CLES

TABLE 2  
PROPERTIES OF THE MAXIMUM-MASS NEUTRON STAR MODELS

Model	$M_{G,\max}/M_\odot$	$M_C/M_\odot$	$\rho_c(\text{g cm}^{-3})$	$P_c(\text{d cm}^{-3})$	$R(\text{km})$	$I(\text{g cm}^2)$	$M_{\text{bind}}/M_\odot$
I H.....	1.85	2.15	$2.28 \times 10^{15}$	$1.26 \times 10^{36}$	9.73	$1.51 \times 10^{45}$	0.294
III H.....	1.73	2.02	$2.69 \times 10^{15}$	$1.58 \times 10^{36}$	8.88	$1.20 \times 10^{45}$	0.292
V H.....	1.65	1.91	$2.47 \times 10^{15}$	$1.00 \times 10^{36}$	9.38	$1.19 \times 10^{45}$	0.256
V N.....	1.76	2.06	$2.49 \times 10^{15}$	$1.33 \times 10^{36}$	9.18	$1.29 \times 10^{45}$	0.301
CLM.....	3.02	3.92	$1.13 \times 10^{15}$	$1.00 \times 10^{36}$	12.9	$5.62 \times 10^{45}$	0.901

NOTE.—“Model” indicates the high-density equation of state used (see text),  $M_{G,\max}$  is the maximum gravitational mass of a stable neutron star,  $M_C$  is the corresponding conserved mass,  $\rho_c$  is the central baryon density ( $= m_n n_b c$ ),  $P_c$  is the central pressure,  $R$  is the radius,  $I$  is the moment of inertia, and  $M_{\text{bind}} = M_C - M_G$  is the binding mass of the maximum mass model.

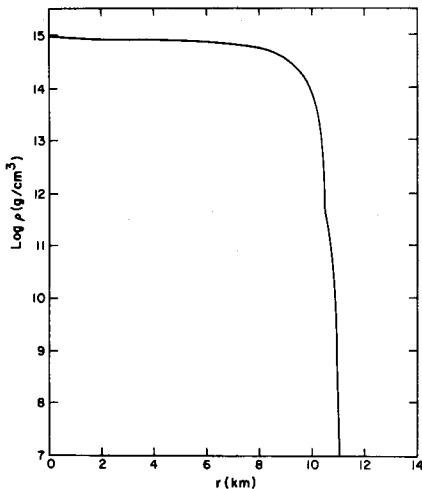


FIG. 5.—Profile of baryon density  $\rho = m_n n_B$  versus radius in an  $M_0 = 1.06 M_\odot$  neutron star model using the equation of state V H.

with  $\rho^* = 5 \times 10^{14} \text{ g cm}^{-3}$ , we can set an upper limit on the mass of a neutron star of  $3 M_\odot$ , assuming that general relativity is the correct theory of gravitation. While this limit is 1.5 to 2 times larger than maximum masses predicted with more realistic equations of state, it is still smaller than the estimated mass of the compact member of the Cygnus X-1 binary system.

Not all recent calculations of the high-density equation of state have given results similar to those obtained above. We cite in particular the calculation of Leung and Wang (1971) which gives a maximum mass of  $0.5 M_\odot$  and maximum moment of inertia  $I_{\max} = 1.0 \times 10^{44} \text{ g cm}^2$  for their preferred equation of state. The results of Leung and Wang differ so much from those obtained by us because they omitted the repulsive interactions among the baryons.

However, we expect that any calculation based on realistic interactions, interactions satisfying criteria (a)-(g) above, will lead to results similar to those we have obtained; the fact that there is such a great separation from the CLM results suggests that (a)-(g), and in particular their implications for the repulsion

in nuclear interactions, represent a strong constraint on the neutron star properties. Further support for this conclusion is provided by a recent calculation by Pandharipande and Smith (1974) of high-density neutron matter, based on the model of Green and Haapakoski (1974). This model accounts for the attraction in the nucleon-nucleon interaction by including a virtual  $\Delta_{33}$  resonance in the intermediate states. Their description of the interaction is different from the models of Bethe and Johnson (1974), having in particular a new saturation mechanism. Most important, they have a satisfactory description for the strength and range of the  $\omega$ -meson repulsion. These calculations have the interesting feature that neutron matter was solid above the density  $n_B = 0.4 \text{ fm}^{-3}$ . Nevertheless, the results for the maximum mass of a neutron star do not differ substantially from our value of  $1.8 M_\odot$  in their most realistic case (Pandharipande 1974).

The only other way (other than drastically changing the underlying interactions) of obtaining different star properties would be to assume that the phase of neutron star matter is not the liquid assumed by Bethe and Johnson (1974). Other candidates are a solid phase (Canuto and Chitre 1973a, b) and a phase containing a condensed  $\pi^-$  mode (Sawyer 1972; Scalapino 1972), to name only two. There exists no compelling evidence to believe that the possible existence of a new phase would much change the star properties. This is supported in part by recent calculations of neutron star models including the effects of pion condensation (Hartle, Sawyer, and Scalapino 1974). However, if the stiffer equations of state of the present work had been used by Hartle *et al.*, the effects of pion condensation would have been even less apparent. We wish to point out that all other things being the same, a phase change could only soften the equation of state. In light of this possibility, the results we have found here represent an improved upper limit on the maximum mass, radius, and moment of inertia, and a lower limit on the maximum central density.

It seems quite firmly established that, if general relativity is accepted as the correct gravitational theory, the maximum mass of a neutron star is less than  $2 M_\odot$ . However, for the present it would be well to bear in mind the comments of § I concerning the possible effects on neutron star masses of other gravitational theories.

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## **Equation of State in the Gravitational Collapse of Stars**

(with G. E. Brown, J. H. Applegate and J. M. Lattimer)  
*Nuclear Phys.* **A324**, 487–533 (1979)

In 1978 when I was visiting the Niels Bohr Institute in Copenhagen for half a year, Gerald Brown, who was stationed there, suggested that we work together on Supernovae of Type II. The main novel point in our theory was that the gravitational collapse can only stop when the density at the center exceeds the density inside a nucleus so that the strong repulsive nuclear forces come into play. We thought at the time that the rebound after collapse would lead to the supernova explosion; this turned out to be wrong. The correct mechanism of expulsion was found in 1982 by James Wilson: the collapsed core contains a lot of energy which is emitted in the form of neutrinos; some of the neutrinos are absorbed by the material at intermediate distances (100–500 km) and their energy propels this material outward.

## EQUATION OF STATE IN THE GRAVITATIONAL COLLAPSE OF STARS

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**Abstract:** The equation of state in stellar collapse is derived from simple considerations, the crucial ingredient being that the entropy per nucleon remains small, of the order of unity (in units of  $k$ ), during the entire collapse. In the early regime,  $\rho \sim 10^{10}\text{--}10^{13} \text{ g/cm}^3$ , nuclei partially dissolve into  $\alpha$ -particles and neutrons; the  $\alpha$ -particles go back into the nuclei at higher densities. At the higher densities, nuclei are preserved right up to nuclear matter densities, at which point the nucleons are squeezed out of the nuclei. The low entropy per nucleon prevents the appearance of drip nucleons, which would add greatly to the net entropy.

We find that electrons are captured by nuclei, the capture on free protons being negligible in comparison. Carrying the difference of neutron and proton chemical potentials  $\mu_n - \mu_p$  in our capture equation forces the energy of the resulting neutrinos to be low. Nonetheless, neutrino trapping occurs at a density of about  $\rho = 10^{12} \text{ g/cm}^3$ . The fact that the ensuing development to higher densities is adiabatic makes our treatment in terms of entropy highly relevant.

The resulting equation of state has an adiabatic index of roughly  $\frac{4}{3}$  coming from the degenerate leptons, but lowered slightly by electrons changing into neutrinos and by the nuclei dissolving into  $\alpha$ -particles (although this latter process is reversed at the higher densities), right up to nuclear matter densities. At this point the equation of state suddenly stiffens, with  $\Gamma$  going up to  $\Gamma \approx 2.5$  and bounce at about three times nuclear matter density.

In the later stages of the collapse, only neutrinos of energy  $\leq 10 \text{ MeV}$  are able to get out into the photosphere, and these appear to be insufficient to blow off the mantle and envelope of the star. We do not carry our description into the region following the bounce, where a shock wave is presumably formed, and, therefore, we cannot answer the question as to whether the shock wave, in conjunction with neutrino transport, can dismantle the star, but a one-dimensional treatment shows the shock wave to be very promising in this respect.

### 1. Introduction

Massive stars ( $M \approx 8\text{--}10 M_\odot$ ) live for  $\sim 10^7 \text{ y}$ , developing peacefully as heavier and heavier nuclear fuels are burned. Burning continues up to  $^{56}\text{Fe}$ , the nucleus with

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the highest binding energy per nucleon. Then, because no further nuclear burning can proceed to create pressure to hold the constituents of the star against gravitational collapse, the end of the star comes with a bang, implosion of the central part into a dense matter core taking a time of the order of 1 sec.

During or following this implosion, the mantle and envelope of the star is thought to be blown off by neutrino transport outward, or by the shock wave formed upon bounce of the central core or by a combination of these two mechanisms, leaving a dense central part which evolves quickly into a neutron star.

The equation of state of the central region of the star during the collapse is obviously important in determining the characteristics and outcome of the implosion. Although determination of the equation of state looks like a formidable problem, considerable simplification can be introduced by the recognition<sup>1,2)</sup> that, after a certain stage in the implosion, neutrinos will be trapped, so that the collapse is adiabatic after this time, and we shall exploit this here.

In earlier calculations<sup>3)</sup> neutrinos produced in neutronization of the core escaped. However, with the advent of weak neutral currents<sup>4,5)</sup>, it was realized<sup>6)</sup> that coherent scattering by nuclei would be effective in giving mean free paths for high-energy neutrinos which were small fractions of the dimensions of the core of the star. Thus, even though travelling between collisions with the speed of light, neutrinos are unable to diffuse out of the central region of the collapsing star in times comparable with collapse time. In a detailed calculation of hydrodynamic collapse, Arnett<sup>7)</sup> examined these questions and came to the conclusion that neutrinos are necessarily trapped for densities higher than  $\rho \approx 10^{12} \text{ g/cm}^3$  if neutrino cross sections are at all comparable with those given by current weak interaction theories<sup>4,5)</sup>.

We shall show in this paper that the crucial feature of the collapse in determining the equation of state is the low entropy involved. At no stage does the entropy, in units of  $k$ , exceed about 1.5 per particle. Since the available number of states goes as  $\exp S/k$ , where  $S$  is the entropy, this implies an astoundingly high order in the system, and this order persists throughout the collapse.

That there is a high order at the beginning of the collapse, which occurs following silicon burning, is understandable. Nucleons are completely in nuclei at this stage, so many ( $\sim 60$ ) nucleons must move in conjunction with each other. The electrons are already highly degenerate at these densities of  $\sim 5 \times 10^9 \text{ g/cm}^3$ , so that their entropy is low,  $\sim 1$  per electron†.

The common hydrodynamic kinetic infall motion of the material is ordered, so that an entropy increase can occur only through the neutronization of the protons. During the early stages of this, low-energy neutrinos can escape freely, and entropy increases. We show that this increase results from: (a) the holes in the electron distribution, which will later be filled in by Auger-like processes, and (b) the deexcitation of nuclear excited states, reached in the electron capture. Neither of

† We measure entropy in units of  $k$ .

these mechanisms gives a large increase in entropy, as we shall show by estimates, and the total increase in entropy *per nucleon* is particularly small, since only a small proportion of the initial electrons ( $\sim 25\%$ ) undergo capture. Thus, up to the stage of neutrino trapping, the entropy per nucleon does not exceed the order of 1.5. Once trapping sets in, the entropy changes only little, as we shall calculate.

Given the low entropy, nucleons have no choice but to remain in nuclei, since drip neutrons would carry a large entropy per particle,  $\sim 8$  at the point of trapping ( $\rho \approx 10^{12} \text{ g/cm}^3$ ), and, consequently, not more than a few percent of the nucleons can be in the drip phase. Nuclei therefore persist up to the point where they begin to touch; i.e., up to nearly nuclear matter density.

The low entropy means that the temperature is kept relatively low during the entire collapse,  $T \leq 6 \text{ MeV}$  right up to the point where nuclei touch. This is an alternative way of understanding that the nucleons are not boiled out of the nuclei on the way in, but only appear once the nuclei merge.

When the nuclei do merge into nuclear matter, the implosion carries this matter to densities of about three times nuclear-matter density, up to  $\rho \sim 8 \times 10^{14} \text{ g/cm}^3$ , before the point of velocity reversal is reached, at which point there is a bounce. This bounce results in the production of a shock wave, and we cannot extend our present description into the region of the shock, but we hope that by giving a simple and realistic equation of state up to the bounce we can remove much of the ambiguity in the initial conditions for the shock.

Our equation of state is exceedingly simple. In densities up to nuclear matter density, the pressure is determined almost completely by the relativistic, degenerate leptons and is consequently that of a relativistic gas of fermions with adiabatic index  $\Gamma$ , slightly less than  $\frac{4}{3}$ , the decrease from  $\frac{4}{3}$  coming chiefly from electron capture. At intermediate stages of the collapse, some nuclei break up into  $\alpha$ -particles and neutrons, and at later stages they recombine. These latter processes have small effects on the equation of state; such effects are well understood, and it would be straightforward to include them in a detailed collapse calculation, so we shall not describe them in detail.

The  $\Gamma \leq \frac{4}{3}$  equation of state for the central zones will persist up to the point where nuclei begin to "feel each other"; i.e., nearly up to nuclear matter densities  $\rho = 2.7 \times 10^{14} \text{ g/cm}^3$ . As the nuclei are squeezed together into nuclear matter, they initially form nuclear matter at normal density, for which the contribution to the pressure from the nucleons is zero. Because of the stiffness of nuclear matter, as it is compressed, the nucleons rapidly take over from the degenerate leptons in determining the pressure and the density cannot be increased very much further before bounce takes place. Throughout much of the region of nuclear matter compression, the increase in nuclear energy is determined by the compression modulus of nuclear matter. The effective  $\Gamma$  in the region above nuclear matter density is  $\sim 2.5$ .

We thus have a very simple and relatively unambiguous collapse scenario in which  $\Gamma$  is slightly less than  $\frac{4}{3}$  over the entire region of densities up to  $\rho \approx 2.7 \times 10^{14} \text{ g/cm}^3$

(nuclear matter density), and then is substantially larger,  $\sim 2.5$ , up to bounce. In a narrow region near nuclear matter density, the sharp edge in the curve for  $\Gamma$  following from the above will be rounded off by effects we do not consider in detail.

Bounce occurs because of the exceedingly stiff equation of state pertaining above nuclear matter density. The bounce is analogous to that of a very stiff spring.

Our description ends at the point of bounce, because we do not include the entropy-producing shock wave. We are able, however, to discuss neutrino diffusion in the absence of shock waves and we show in appendix C that the diffusion rate is too slow for the neutrinos by themselves to blow off the mantle and envelope of the star. A one-dimensional treatment of the shock wave shows it to be very promising in this respect, although a three-dimensional calculation would be necessary to establish this.

## 2. Electron fraction, energy and entropy

Collapse begins, following Si burning, when the mass of the core of the star exceeds the Chandrasekhar limit:  $\sim 1.2 M_{\odot}$ . We assume the core develops independently of the more massive mantle and envelope; this is reasonable to the extent that the characteristic time for Si burning is long compared with the time for collapse of the central core.

We begin from the initial central conditions of Arnett<sup>7)</sup>:

$$\rho_c = 3.7 \times 10^9 \text{ g/cm}^3, \quad T_c = 8.0 \times 10^9 \text{ K} = 0.69 \text{ MeV}, \quad (1)$$

which are supposed to pertain following Si burning.

There is general agreement on the initial number of electrons per baryon  $Y_e^{(i)}$  and that the presence of the degenerate electron gas with initial chemical potential  $\mu_e = 6 \text{ MeV}$  pushes the nuclei toward neutron rich isotopes, such that

$$\hat{\mu} \equiv \mu_n - \mu_p = \mu_e, \quad (1.1)$$

there being plenty of time to establish  $\beta$ -equilibrium. Arnett<sup>7)</sup> arrived at  $Y_e^{(i)} = 0.41$  enforcing hydrostatic equilibrium at the end of Si burning. Weaver, Zimmerman and Woosley<sup>8)</sup> calculate in detail the nuclear transformations during Si burning and conclude, as Arnett, that a lot of electron capture takes place already in the pre-supernova stage, especially because this stage (in their calculation) lasts fairly long, several days. They find that "the composition is dominated by very neutron-rich species such as  $^{48}\text{Ca}$ ,  $^{66}\text{Ni}$ ,  $^{50}\text{Ti}$ ,  $^{54}\text{Cr}$  near the center of the star" and gradually shifts to less neutron-rich species farther out. These species have, respectively,  $Y_e = 0.417, 0.424, 0.440$  and  $0.444$ , and, accordingly, the central electron abundance found by Weaver *et al.*<sup>8)</sup> is  $Y_e^{(i)} = 0.427$  (for a star of  $15 M_{\odot}$ ). The favored nuclear species listed above mostly have at least one closed shell,  $N = 28$  (Ca, Ti),  $Z = 28$  (Ni) or  $Z = 20$  (Ca), which explains their high abundance in the stellar matter.

Our formula (4.4), which we shall give later as representing the best overall fit to  $\mu_n - \mu_p$  taking into account bulk, surface and Coulomb energies, would predict an initial  $Y_e$  between 0.41 and 0.42 (see table 1) but we shall show in appendix A, by comparison with binding energies of the Fe isotopes, that our bulk contribution to  $\mu_n - \mu_p$  appears to be a bit too small in this region (or the surface contribution is too large), so that  $Y_e^{(i)} \approx 0.42$  seems reasonable. We shall adopt this value. The precise  $Y_e^{(i)}$  we choose is important only for estimating the entropy increase during the process of electron capture and will not be critical for our results.

TABLE 1  
 $\hat{\mu} = \mu_n - \mu_p$  as function of  $Y_e$

$Y_e$	$\omega_{\text{surf}}$ eq. (4.1)	$\bar{A}$	$\hat{\mu} = \mu_n - \mu_p$ eq. (4.4)	Epstein's empirical $\hat{\mu}_*$ eq. (4.6)	$\frac{d\hat{\mu}}{d Y_e}$ (eq. (12.1))
0.48	18.1	69			-170
0.464	17.9	73	-2.7*	-0.6	
0.46	17.9	74	-2.0	0	-177
0.44	17.6	80	1.7	2.88	-184
0.42	17.2	86	5.6	5.76	-191
0.40	16.7	91	9.5	8.6	-198
0.38	16.1	98	13.7	11.5	-206
0.36	15.4	105	18.0	14.4	-214
0.34	14.6	111	22.4	17.3	-223
0.32	13.7	118	27.1	20.2	-232
0.30	12.8	125	31.7	23.0	-240
0.28	11.8	132	36.6	25.9	-250
0.26	10.7	137	41.6	28.8	-259
0.24	9.6	147	47.0	34.6	-269
0.22	8.5	154	52.4	37.4	-279
0.20	7.4	163	58.1		-289

The density  $\rho = 10^{12}$  g/cm<sup>3</sup> is assumed in evaluating  $\bar{A}$ , eq. (5).

\* This negative value is an indication that we should increase the bulk symmetry energy (or decrease the magnitude of the surface symmetry energy) as discussed in appendix A.

The initial entropy per nucleus for translational motion is given by

$$\frac{1}{N} \frac{S}{k} = \frac{5}{2} + \ln \left[ \frac{V}{N} \left( \frac{M k T}{2 \pi \hbar^2} \right)^{\frac{3}{2}} \right] = 16.70, \quad (2)$$

where  $N$  is the number of nuclei in volume  $V$ , and  $M$  the average mass, which we take to be that of <sup>56</sup>Fe. To this we add the entropy of the excited states of the nucleus and the entropy due to the  $\alpha$  particles and neutrons present due to thermal dissociation of nuclei. At the temperature and density (1) the  $\alpha$ 's and neutrons

contribute 3.6 and the excited nuclear states contribute 4.8. Thus the initial entropy per nucleon, obtained by dividing by 56, is

$$(S/k)_{\text{per nucleon}} = 0.45. \quad (2.1)$$

For the electrons, the Fermi energy is initially  $\mu_e = 6.0 \text{ MeV} \approx 8.6 kT$ . Thus,

$$(S/k)_{\text{per electron}} = \pi^2 \frac{kT}{\epsilon_F} \approx 1.15, \quad (2.2)$$

and this gives a total entropy per nucleon of

$$(S/k)_{\text{total}} = 0.45 + 0.48 = 0.93. \quad (2.3)$$

Entropy will increase during the development of the core up to neutrino trapping ( $\rho \approx 10^{12} \text{ g/cm}^3$ ) through electron capture†. The electron capture increases entropy, firstly because it occurs in matter that is not in beta equilibrium, and secondly because electron captures lead to excited states of the daughter nuclei which decay then to the ground state, mainly by  $\gamma$ -emission. However, escaping neutrinos will carry off a large fraction of the entropy. To show this we begin with a result from thermodynamics

$$dE + P dV = \sum \mu_i dN_i + T dS = dQ, \quad (3)$$

where the sum goes over electrons, protons and neutrons (and neutrinos, if they are trapped). Here  $E$  and  $S$  are the total internal energy and entropy and  $N_i$  is the total number of particles of species  $i$ .  $Q$  is the total heat lost or gained during the collapse. In electron capture  $dN_n = -dN_e = -dN_p$  ( $= dN_\nu$ , if neutrinos are trapped). We are interested in the case in which neutrinos are not trapped and freely escape so that  $dQ$  will be  $dN_e$  times some fraction of the maximum energy available for electron capture,  $\Delta$ . In appendix F we show this fraction to be about  $\frac{3}{5}$ . As long as neutrinos are not trapped  $\Delta = \mu_e - \hat{\mu} - \Delta_n$ , where  $\Delta_n$  is the excitation energy of the daughter nucleus, shown in appendix B to be of order 3 MeV. Eq. (3) now becomes

$$T(dS)_{\text{per nucleon}} = -dY_e[\mu_e - \hat{\mu} - \frac{3}{5}\Delta], \quad (3.1)$$

† Entropy increase proceeds only through the weak interactions, since the various phases are in equilibrium under the strong interactions. Although relevant times for the important part of collapse are only milliseconds, this is a long time compared with equilibration times of the strong and electromagnetic interactions. Indeed, we shall find that even the weak interactions, which are a factor of  $\sim 10^{12}$  weaker than the strong interactions, equilibrate by densities of  $\rho = 10^{12} \text{ g/cm}^3$  to the extent that entropy production beyond this density in the collapse is small, so it is clear that we have many orders of magnitude in hand when we maintain that the system is in equilibrium as far as the strong interactions are concerned.

or

$$T(dS)_{\text{per nucleon}} = -dY_e \left[ \frac{2}{5}(\mu_e - \hat{\mu}) + \frac{3}{5}\Delta_n \right], \quad (3.2)$$

which clearly shows the two contributions to entropy generation. We calculate later (eq. (15.2)) that  $Y_e$  at trapping is about 0.31 so that  $\Delta Y_e \approx -0.11$ , and from eq. (14.3) we find  $\Delta$  to be about 6 MeV. The average temperature during this part of the collapse is  $T = 1.4$  MeV (see table 10). Thus  $0.11(9/1.4) = 0.71$  units of entropy per nucleon are generated by electron capture (the excitation energy adds to the amount the system is out of  $\beta$ -equilibrium), but  $0.11 \frac{3}{5}(6/1.4) = 0.28$  units of entropy are carried off by neutrinos. The difference, 0.43, is the total entropy per nucleon produced up to neutrino trapping. Adding this to (2.3) we would have a total entropy per nucleon of 1.36. We adopt the value of

$$(S/k)_{\text{per nucleon}} = 1-1.5, \quad (3.3)$$

as our estimate of the final entropy, although our arguments and results would be little changed were the entropy  $\sim 50\%$  higher. Detailed calculations of entropy production will be given later (see appendix F) and give numbers which agree with our estimates. In particular, table 9 gives results calculated under the assumption of no neutron drip, and the entropy increase there is shown to be smaller than our above estimates. In the more realistic calculations of table 10, which include neutron drip, the entropy for  $Y_e = 0.31$  is in line with our above estimate of  $S/k \sim 1.3$ , and even for  $\rho_{10} = 107.5$ ,  $S/k = 1.48$ , within the range of eq. (3.3).

The value of  $Y_e^{(t)}$  which was important in this calculation, is obtained from the difference between the chemical potentials of neutron and proton  $\hat{\mu} = \mu_n - \mu_p$ . We shall find in the next section that this  $\hat{\mu}$  stays close to the electron chemical potential  $\mu_e$ , which in turn depends mainly on the density of matter,  $\rho$ . We shall use the following expression for  $\hat{\mu}$ , taken from Baym, Bethe and Pethick<sup>9</sup> (BBP):

$$\hat{\mu} = \mu_n - \mu_p = -\frac{1}{A} (\partial W_N / \partial Y_e)_{\rho_N, V_N, u}, \quad (4)$$

where  $W_N$  is the total energy of a single nucleus:

$$W_N(Y_e, \rho_N, V_N, u) = W_{\text{bulk}} + \alpha(Y_e) V_N^{\frac{2}{3}} + \beta Y_e^2 \rho_N^2 V_N^{\frac{5}{3}} (1 - \frac{3}{2}u^{\frac{1}{3}} + \frac{1}{2}u). \quad (4.1)$$

These three terms are the nuclear bulk energy, surface energy and Coulomb energy respectively, and  $\rho_N$  is the density inside a nucleus,  $V_N$  is the nuclear volume and  $u$  is the fraction of the total volume occupied by nuclei so that  $A = \rho_N V_N$  and  $u = \rho/\rho_N$ . For  $\alpha$  we use the results of Ravenhall, Bennett and Pethick<sup>12</sup>) who calculated the surface energy as a function of  $Y_e$ . If the surface energy in MeV is expressed as  $\omega_{\text{surf}} A^{\frac{2}{3}}$  so that  $\alpha = \omega_{\text{surf}} \rho_N^{\frac{2}{3}}$ , a fit to ref. <sup>12</sup>) in the range  $0.25 \leq Y_e \leq 0.5$  gives

$$\omega_{\text{surf}} = 290 Y_e^2 (1 - Y_e)^2. \quad (4.2)$$

If the Coulomb energy in MeV is expressed as  $\omega_{\text{Coul}} A^{\frac{5}{3}}$ , we have, from BBP:

$$\omega_{\text{Coul}} = 0.75 Y_e^2 (1 - 0.236 \rho_{12}^{\frac{1}{3}} + 0.00194 \rho_{12}), \quad (4.3)$$

where  $\rho_{12}$  is the density in units of  $10^{12} \text{ g/cm}^3$ . Evaluating the derivative in eq. (4) gives

$$\hat{\mu} = 250(0.5 - Y_e) - \omega_{\text{surf}} A^{-\frac{1}{3}} \left( \frac{1}{Y_e} + \frac{2}{Y_e} \frac{1 - 2Y_e}{1 - Y_e} \right). \quad (4.4)$$

The first term comes from the bulk symmetry energy taken from BBP. The second term represents surface and Coulomb corrections. In obtaining eq. (4.4) we have used the BBP prescription that the nuclear surface energy be twice the Coulomb energy.

$$\omega_{\text{surf}} A^{\frac{2}{3}} = 2\omega_{\text{Coul}} A^{\frac{5}{3}}. \quad (4.5)$$

As we shall point out in appendix A, there is some ambiguity in determining  $\hat{\mu}$  empirically from nuclear masses, since surface symmetry energies can be changed in such a way as to compensate for rather large changes in the volume symmetry energy and the result can be rather different for  $\hat{\mu}$  in the region far from stability. An alternative expression for  $\hat{\mu}$  has been determined completely empirically by Epstein<sup>11</sup>). He examines the energies (mass excess) of observed, neutron-rich nuclei and compares them with their most stable isobars; by differentiation,  $\hat{\mu}$  is obtained. He finds that the nuclei most favorable for high neutronization (such as <sup>48</sup>Ca, <sup>66</sup>Ni, <sup>132</sup>Sn) can be fitted by

$$\hat{\mu} = 144 (0.46 - Y_e). \quad (4.6)$$

For  $Y_e \leq 0.35$  this gives somewhat smaller  $\hat{\mu}$ 's than we obtain from eq. (4.4). In table 1 we report values from Epstein's formula (4.6), as well as from eq. (4.4). Employing the generally smaller values from eq. (4.6) would not change our results appreciably.

We have found that the expression

$$\hat{\mu} = 207 (0.45 - Y_e)(1.32 - Y_e), \quad (4.7)$$

reproduces accurately results of our complete expression (4.4).

Formulae deduced from empirical binding energies may not be directly applicable to our problem. Whereas the nuclei most bound, because of shell effects and pairing, will be formed in the initial stages as long as the temperature is low; as soon as the temperature increases, nuclei will be in highly excited states, and there will be little influence from shell effects and pairing. For the temperature of 1.9 MeV relating to Arnett's<sup>7</sup>) zone 13 which we often use as an example, the excitation energy of a nucleus with  $A \approx 56$  is  $U = 24$  MeV, computed from our later eq. (20.3). For this

excitation energy such a nucleus has a level density of  $2 \times 10^7$  levels per MeV. Thus, shell effects and pairing in the ground state will have little to do with the evolution of the collapse and the Fermi gas treatment of BBP [ref. <sup>9</sup>] and of ref. <sup>10</sup>) is appropriate.

A more detailed argument for this conclusion goes as follows: In nuclei with one or two closed shells, the shell closure lowers the ground state energy of the system through additional binding effects, but leaves the level density at any appreciable temperature at roughly the value appropriate for odd-odd nuclei. The excitation energy of the closed shell nucleus above the ground state would be higher, but then the additional binding of the ground state should be subtracted before calculating level densities. A similar discussion pertains to effects from pairing.

To conclude this section, we estimate the most likely atomic weight as a function of  $Y_e$ , which is needed to determine  $\hat{\mu}$  and the neutrino mean free path eq. (16). For this we simply use the BBP condition, eq. (4.5), which gives, after neglecting a small term,

$$A = 194(1 - Y_e)^2(1 - 0.236\rho_{12}^{\frac{1}{3}})^{-1}. \quad (5)$$

The resulting values of  $A$  are given in table 1 for  $\rho = 10^{12}$  g/cm<sup>3</sup>. It is seen that in the important range around  $Y_e = 0.3$ ,  $A$  is roughly twice as big as for Fe.

The neutron chemical potential can be found, following BBP eq. (2.10):

$$\mu_n = (\partial W_N / \partial A)_{Z, V_N, u}, \quad (5.1)$$

which we cast as

$$\mu_n = \frac{1}{V_N} \left( \frac{\partial W_N}{\partial \rho_N} \right)_{Y_e, V_N, u} - \frac{Y_e}{A} \left( \frac{\partial W_N}{\partial Y_e} \right)_{\rho_N, V_N, u}, \quad (5.2)$$

since  $W_N$  is an explicit function of  $V_N$ ,  $\rho_N$ ,  $Y_e$  and  $u$ . We obtain

$$\mu_n = -16 + 125(0.5 - Y_e) - 150(0.5 - Y_e)^2 - 2\omega_{\text{surf}} A^{-\frac{1}{3}} \frac{1 - 2Y_e}{1 - Y_e}, \quad (5.3)$$

where the first three terms come from the bulk energy taken from BBP. At zero temperature, neutron drip occurs when  $\mu_n = 0$ , or from eq. (5.3), when  $(Y_e)_{\text{drip}} \approx 0.30$ . This compares with BBP, who found  $(Y_e)_{\text{drip}} = 0.315$ . Whereas our value  $Y_e^{(t)} = 0.31$ , to be derived in the next section, is near  $(Y_e)_{\text{drip}}$ , so that neutrino trapping occurs in our calculations near the neutron drip, some neutron drip would in no way be catastrophic, since the leptons would still give the overwhelming contribution to the pressure below nuclear matter density. (Recall that the contribution of a free neutron to the pressure will be  $kT$ . For our maximum temperature of 6 MeV, before nuclei merge, this is small compared with the average contribution per electron of  $\frac{1}{4}\mu_e$ ,  $\mu_e$  being about 100 MeV in the region important for collapse. Thus, the number of drip neutrons could be comparable with the number of electrons with little modification in our results.) At finite temperatures, neutrons begin to drip at

larger  $Y_e$  values, however. To account for them, the  $Y_e$  of eqs. (4) through (5.3) should be replaced by  $x = Z/A$ , related to  $Y_e$  by

$$x = Y_e/(1 - X_n), \quad (5.4)$$

where  $X_n$  is the drip neutron mass fraction. For the low entropies of our calculations,  $X_n \leq 0.2$  at densities below  $10^{12} \text{ g/cm}^3$ . Thus drip neutrons have little effect on our calculation of  $Y_e^{(t)}$  (see appendix F).

### 3. Electron capture rate

We now discuss the rate of electron capture and "neutronization" of the nuclear matter. In the literature considerable complication is introduced involving strength functions for electron capture, networks of nuclei, etc. We believe that for general features these complications are unnecessary and that a description based on the shell model is both simpler and more accurate. Capture on free protons is assumed to play a dominant role in many earlier descriptions. Because of the paucity of these, (see table 4) they are actually unimportant, except possibly just in the beginning of collapse where the electron chemical potential of 6 MeV may be insufficient for the electrons to supply the excitation energy necessary in the daughter nucleus to find the main shell-model strength†.

In this section we shall use the Fermi gas model for the nuclei and give in appendix B the relation of the Fermi gas model to the shell model. The latter will vary from nucleus to nucleus; we give arguments that the Fermi gas model should reproduce average features.

The cross section for electron capture, with neutrino emission, on a proton at rest is‡†

$$\sigma = 1.18 \times 10^{-44} (\epsilon_\nu/m_e)^2 \text{ cm}^2. \quad (6)$$

Not all electrons and protons will be able to participate in the capture, however. Among the protons, only those near the maximum (Fermi) energy  $\mu_p$  will be effective; the number of these in an energy interval  $d\epsilon_p$  is

$$\frac{mk_F d\epsilon_p}{\frac{1}{3}k_F^3} \quad (\epsilon_p < \mu_p), \quad (6.1)$$

where  $m$  is the mass of a nucleon. The energy relation in the electron capture is

$$\epsilon_e + \epsilon_p = \epsilon_n + \epsilon_\nu. \quad (6.2)$$

† Even if free protons are responsible for the electron capture, they have to be replenished from nuclei. The resulting relation between  $\hat{\mu}$  and  $\mu_e$  will then be quite similar to (12.6) albeit with a different coefficient.

‡† Derived from the weak coupling constant  $g_V = 1.00 \times 10^{-5} m^{-2}$ , where  $m$  is the nucleon mass, and the ratio of axial vector to vector coupling constants  $g_A/g_V = 1.25$ .

Assuming low temperature, in accord with the low entropy deduced in sect. 2, we must have

$$\epsilon_e = \mu_e - \Delta_e, \quad \epsilon_p = \mu_p - \Delta_p, \quad \epsilon_n = \mu_n + \Delta_n, \quad (6.3)$$

where the  $\mu$ 's are the chemical potentials (Fermi energies) and the  $\Delta$ 's are positive quantities. In particular,  $\Delta_n$  is the excitation energy in the daughter nucleus† which is needed to find the main shell-model strength for the  $\beta$ -transition. In appendix B, we show that

$$\Delta_n \approx 3 \text{ MeV}. \quad (6.4)$$

The other three quantities we combine, thus

$$\Delta = \Delta_e + \Delta_p + \epsilon_n, \quad (6.5)$$

and we also introduce

$$\hat{\mu} = \mu_n - \mu_p. \quad (6.6)$$

Then the energy relation (6.2) becomes

$$\mu_e = \hat{\mu} + \Delta + \Delta_n. \quad (6.7)$$

Using these notations, the energy-averaged proportion of the total number of electrons and protons which can participate, with inclusion of the energy factor  $\epsilon_\nu^2/m_e^2$  from eq. (6), is

$$X = \int_0^\Delta \frac{\epsilon_\nu^2}{m_e^2} d\epsilon_\nu \int^{\Delta-\epsilon_\nu} \frac{d\epsilon_p}{k_t^2/3m} \frac{3\epsilon_e^2}{\mu_e^3}, \quad (7)$$

where, by our definition,

$$\epsilon_e = \mu_e - (\Delta - \Delta_p - \epsilon_\nu). \quad (7.1)$$

It will turn out that in general  $\Delta_e \ll \epsilon_e$ ; i.e., the electrons must come near the top of the Fermi distribution. We can set  $\epsilon_e \approx \mu_e$  and we easily obtain, upon integration

$$X = \frac{1}{4} \frac{\Delta^4}{m_e^2 (k_t^2/3m) \mu_e}. \quad (7.2)$$

Consequently, the time rate of change of the electron proportion is

$$\frac{dY_e}{dt} = -X\rho (\text{in g/cm}^3) Y_e N_0 c \sigma_0 Y_e, \quad (8)$$

† It could be argued that  $\Delta_n + \Delta_p$  is the excitation energy. In this case,  $\Delta$  in (15) etc. will be somewhat smaller.

where  $N_0$  is Avagadro's number ( $6 \times 10^{23}$ ). Here  $\rho Y_e N_0$  is just the number† of protons/cm<sup>3</sup>. Using the cross section from eq. (6), we obtain

$$\frac{dY_e}{dt} = -2.12 X \rho_{10} Y_e^2 \text{ sec}^{-1}, \quad (8.1)$$

where  $\rho_{10}$  is the density measured in units of  $10^{10}$  g/cm<sup>3</sup>. In deriving this equation we have assumed that we are at sufficiently low energies that the neutrinos can escape freely; i.e., there is no blocking.

Since  $\rho$  occurs as a factor on the right hand side of (8.1) we would like to have an equation expressing  $Y_e$  as function of the density  $\rho$ ; to this end, we try to obtain  $\rho$  as a function of  $t$ . Epstein, Nørgaard and Bond<sup>14</sup>), in fitting Arnett's collapse calculation<sup>7</sup>) find‡

$$\frac{d(\ln \rho)}{dt} = 19 \rho_{10} \quad (9)$$

This formula gives a collapse rate which exceeds the free-fall rate slightly above  $\rho = 10^{12}$  g/cm<sup>3</sup>. We find this to be unreasonable because of the following argument.

Homologous collapse of a star in free fall gives a collapse rate

$$\frac{d(\ln \rho)}{dt} = 224_{10}^{\frac{1}{2}}. \quad (9.1)$$

This would be the correct rate of development were all of the leptons removed from a core of mass equal to the Chandrasekhar limit. However, at no point during the collapse have more than 26% of the leptons initially present disappeared (we take  $Y_e^{(i)} = 0.42$  and shall find  $Y_e^{(f)} = 0.31$ ), so the leptons offer considerable degeneracy pressure to resist collapse. In fact, since the pressure for a gas of relativistic degenerate Fermions is proportional to  $n^{\frac{4}{3}}$ , where  $n$  is the number density, a fraction

$$F = \frac{4}{3} \frac{Y_e^{(i)} - Y_e}{Y_e^{(i)}}, \quad (9.2)$$

of the lepton support pressure has been removed at the stage of collapse corresponding to a given  $Y_e$ . In our calculations,  $F$  never exceeds 35%, since our final  $Y_e$  is 0.31.

With retention of most of the leptons, the equation for homologous collapse of a core of radius  $R$  would read

$$\frac{d^2 R}{dt^2} = -\frac{GM}{R^2}(F), \quad (9.3)$$

† Of course, these protons are inside nuclei, as discussed earlier in this section.

‡ These authors give several values for the constant we write as 19 in eq. (9); their central value, used here, corresponds closely to our conditions. In an independent fit, before we knew of their work, we obtained an identical equation with 25 instead of 19.

where  $M$  is the mass of the core. Solution of this equation for  $F = 1$  and use of

$$\rho = M/\frac{4}{3}\pi R^3. \quad (9.4)$$

leads to the free-fall eq. (9.1). Eq. (9.3) would be difficult to solve in detail, because  $Y_e$ , and therefore  $F$ , is a function of  $t$ . However, if  $F$  is constant, the result is

$$\frac{d(\ln \rho)}{dt} = 224(\rho_{10}F)^{\frac{1}{2}}. \quad (9.5)$$

Since we have seen that  $F$  never exceeds 0.35, we take the average  $F$  to be 0.20 and get

$$\frac{d(\ln \rho)}{dt} = 100\rho_{10}^{\frac{1}{2}}. \quad (10)$$

This rate differs appreciably from that given in eq. (9).

In any case, it must be made clear just which density is to be used on the right-hand side of (10), so we go into a more detailed discussion of homologous collapse.

Collapse can be homologous only in the region where the sound velocity exceeds the infall velocity, since different parts of the core must be able to "communicate" with each other if they are to collapse together. From Arnett's<sup>7)</sup> fig. 5, this defines the radius of the homologous core as  $\sim 40$  km, roughly that of his zone 12. Taking  $r_k$  and  $u_k$  to be the radius and velocity of zone  $k$ , and

$$\frac{d(\ln \rho)}{dt} = -3 \frac{u_k}{r_k}, \quad (10.1)$$

to define a rate for this zone,  $k = 12$ , we find

$$\left( \frac{d(\ln \rho)}{dt} \right)_{\text{zone } 12} = 1166 \text{ sec}^{-1}. \quad (10.2)$$

On the other hand, for Arnett's zone 12,  $\rho_{10} = 135$ , so we would obtain  $1162 \text{ sec}^{-1}$  from eq. (10). The agreement is good, and serves to specify the density  $\rho$  in eq. (10) as the density at the outer edge of the homologous sphere. Taking zone 8, right in the middle of the core, we find  $-3u_k/r_k = 933 \text{ sec}^{-1}$ , not greatly different from the value for zone 12, indicating that the core really does collapse homologously.

Combining eqs. (8.1) and (10), we obtain

$$\frac{d Y_e}{d(\ln \rho)} = -\frac{2.12}{100} X \rho_{10}^{\frac{1}{2}} Y_e^2, \quad (11)$$

giving the development of  $Y_e$  with  $\rho$ .

The factor  $X$  depends sensitively on  $\Delta$ , eq. (7.2), i.e., on the difference  $\mu_e - \hat{\mu}$ , cf. (6.7). It is therefore desirable to convert (11) into an equation depending on the symmetry energy  $\hat{\mu} = \mu_n - \mu_p$  by writing  $Y_e$  in terms of  $\hat{\mu}$ . Combining eqs. (4.4) and

(5) and dropping the insignificant factor involving the density in the latter equation (we are interested now only in densities less than  $\sim 10^{12}$  g/cm<sup>3</sup>), one has

$$\hat{\mu} = 250 (0.5 - Y_e) - 50 Y_e (1 - Y_e)^{\frac{1}{3}} (3 - 5 Y_e). \quad (12)$$

Taking the derivative,

$$\frac{d\hat{\mu}}{dY_e} = -250 - \frac{150}{(1 - Y_e)^{\frac{2}{3}}} \left( 1 - \frac{14}{3} Y_e + \frac{35}{9} Y_e^2 \right). \quad (12.1)$$

In table 1 we tabulate  $d\hat{\mu}/dY_e$  from this equation as a function of  $Y_e$ . One sees that  $d\hat{\mu}/dY_e$  is constant in the range  $0.2 < Y_e < 0.4$  to within 20%. Since we shall see that our results are affected by only the  $\frac{1}{4}$  power of this constant, we assume henceforth that  $d\hat{\mu}/dY_e$  follows the bulk behavior,

$$\frac{d\hat{\mu}}{dY_e} = -250. \quad (12.2)$$

Using this, we have

$$\frac{dY_e}{d(\ln \rho)} = -\frac{1}{250 \text{ MeV}} \frac{d\hat{\mu}}{d(\ln \rho)}. \quad (12.3)$$

Since  $\rho$  can be expressed in terms of  $Y_e$  and  $\mu_e$ ,

$$\rho = C\mu_e^3/Y_e, \quad (12.4)$$

with  $C$  a constant, and since it can be shown that the rate of change of  $\ln Y_e$  is at most 10% of that of  $\ln \mu_e^3$ , we have

$$\frac{d\hat{\mu}}{d(\ln \rho)} \approx \frac{\mu_e}{3} \frac{d\hat{\mu}}{d\mu_e} = -250 \text{ MeV} \frac{dY_e}{d(\ln \rho)}. \quad (12.5)$$

where we have used eq. (12.2) in the last step. Using eq. (11) we obtain, then,

$$\frac{d\hat{\mu}}{d\mu_e} = \frac{6.36}{100} \frac{250 \text{ MeV}}{\mu_e} X \rho_{10}^{\frac{1}{2}} Y_e^2. \quad (12.6)$$

Taking  $k_t^2/m = 80$  MeV in  $X$ , eq. (7.2), and expressing all energies in MeV, we have, finally,

$$\frac{d\hat{\mu}}{d\mu_e} = 0.57 \rho_{10}^{\frac{1}{2}} Y_e^2 \frac{\Delta^4}{\mu_e^2}. \quad (13)$$

This important equation gives the rate at which  $\hat{\mu} = \mu_n - \mu_p$  follows  $\mu_e$ . We note once more that, cf. (6.7),

$$\Delta = \mu_e - \hat{\mu} - \Delta_n, \quad (13.1)$$

where  $\Delta_n$  was previously shown to have the fixed value of 3 MeV.  $Y_e$  is expressible in terms of  $\hat{\mu}$ , eq. (12), and  $\rho$  in terms of  $\mu_e$ , eq. (12.4). Thus (13) is a differential

equation for  $\hat{\mu}$  in terms of  $\mu_e$ . It can be solved by direct numerical integration†. Regardless of the initial conditions on  $\mu_e$  and  $\hat{\mu}$ , the results are in agreement with the following simple consideration.

As the density, and hence  $\mu_e$ , increases, the right-hand side of (13) would become very large if  $\Delta$  were a constant fraction of  $\mu_e$ . The differential equation then would indicate that  $\hat{\mu}$  increases much faster than  $\mu_e$ , but this is impossible because of (13.1). Hence  $\Delta/\mu_e$  must decrease with increasing  $\mu_e$  (density), which means that  $\hat{\mu}$  follows  $\mu_e$  more and more closely. Therefore,

$$\frac{d\hat{\mu}}{d\mu_e} \rightarrow 1 \quad \text{for large } \mu_e. \quad (13.2)$$

Setting the left-hand side of (13) to one gives

$$\Delta = \frac{1.15}{\rho_{10}^{\frac{1}{8}}} \sqrt{\frac{\mu_e}{Y_e}}. \quad (14)$$

The factor  $\rho^{\frac{1}{8}}$  would not have occurred in the denominator had we used the collapse rate (9) rather than (10); its presence expresses the fact that with our slower collapse rate at high densities we are closer to equilibrium between electron capture and  $\beta$ -decay, so that  $\mu_n - \mu_p$  is closer to  $\mu_e$ .

If we insert in (14) the value of  $\mu_e$ ,

$$\mu_e = 11.1(\rho_{10} Y_e)^{\frac{1}{3}} \text{ MeV.} \quad (14.1)$$

we obtain

$$\Delta = 3.83 Y_e^{-\frac{1}{3}} \rho_{10}^{\frac{1}{24}}. \quad (14.2)$$

Using our standard value  $Y_e = 0.31$ ,

$$\Delta = 5.7 \rho_{10}^{\frac{1}{24}}. \quad (14.3)$$

The dependence on the density  $\rho_{10}$  is extremely weak; even at  $\rho = 10^{12} \text{ g/cm}^3$ ,  $\Delta = 6.9 \text{ MeV}$ . The total lag  $\mu_e - \hat{\mu}$  is  $\Delta + \Delta_n$ , eq. (13.1), and hence about 10 MeV. Going to a lower density, like  $\rho_{10} = 1$ , (14.3) still gives a large  $\Delta$ , so  $\mu_e - \hat{\mu}$  is quite large (see eq. (13.1)) which would mean that  $\hat{\mu}$  lags considerably behind  $\mu_e$  at low density. Our procedure is not applicable to low density, because: (a) the collapse rate is slower than eq. (10), and (b)  $d\hat{\mu}/d\mu_e < 1$ .

For zone 12 of Arnett<sup>7</sup>)  $\rho_{10} = 135$ ,  $\mu_e = 39.0$  and  $Y_e = 0.32$ . Using eq. (14),

$$\Delta = 6.88 \text{ MeV.} \quad (15)$$

From eq. (13.1) and using  $\Delta_n = 3 \text{ MeV}$  we find

$$\mu_n - \mu_p = 29.1 \text{ MeV,} \quad (15.1)$$

† We are indebted to R. Epstein for doing such an integration. We have independently repeated this integration; results are given in table 2.

TABLE 2  
Values of  $Y_e$  and  $\hat{\mu} = \mu_n - \mu_p$  as functions of density  $\rho$

$\log \rho$	$Y_e$	$\mu_e$ (MeV)	$\hat{\mu}$ (MeV)	$\frac{d\hat{\mu}}{d\mu_e}$	$\Delta =$ $\mu_e - \hat{\mu} - \Delta_n$	$\Delta$ from eq. (14)
9.0	0.420	3.86	4.27	0.03	-3.41	4.65
9.5	0.420	5.66	4.33	0.03	-1.67	4.87
10.0	0.420	8.31	4.42	0.03	0.89	5.11
10.25	0.420	10.07	4.50	0.08	2.57	5.24
10.50	0.418	12.20	4.90	0.35	4.30	5.37
10.75	0.411	14.78	6.40	0.76	5.38	5.54
11.0	0.399	17.61	8.82	0.92	5.79	5.73
11.25	0.384	21.06	12.08	0.95	5.98	5.94
11.50	0.366	25.10	15.96	0.96	6.14	6.18
11.75	0.346	29.85	20.53	0.96	6.32	6.45
12.0	0.324	35.39	25.88	0.97	6.51	6.75
12.13*	0.311	38.58	28.97	0.97	6.61	6.94

Also tabulated are  $d\hat{\mu}/d\mu_e$  from eq. (13) and  $\Delta = \mu_e - \hat{\mu} - \Delta_n$ . In the last column, the asymptotic values of  $\Delta$  from eq. (14) are given. Remember that  $\Delta$  is also the maximum neutrino energy  $(\epsilon_\nu)_{\max}$ , and  $\Delta_n$  is the assumed excitation energy of the daughter nucleus (see appendix B).

\*  $\rho = 1.35 \times 10^{12}$  g/cm<sup>3</sup> (Arnett's zone 12).

for this zone. Using eq. (12), this can be translated into a  $Y_e$  consistent with our development,

$$Y_e = 0.31. \quad (15.2)$$

This is just the value of  $Y_e$  for this density obtained by numerical integration of eq. (11) (see table 2). To be consistent, we should use this  $Y_e$  back in eq. (14) and also correct  $\mu_e$ , to obtain

$$\mu_e = 38.5 \text{ MeV}, \quad \Delta = 6.92 \text{ MeV}. \quad (15.3)$$

As can be seen, there is considerable stability in these numbers.

After making the preceding arguments in this section, we checked their validity by direct computations. Eq. (11) can be solved straightforwardly by numerical integration. Following our earlier discussion, the initial value of  $Y_e$  is  $Y_e^{(i)} = 0.42$  at  $\rho = 3.7 \times 10^9$  g/cm<sup>3</sup>. The quantity  $\Delta$  can be evaluated from eq. (6.7),  $\hat{\mu}$  being given as a function of  $Y_e$  by eq. (4.4) and  $\mu_e$  can be calculated from  $Y_e$  and  $\rho$  (see our eq. (14.1)). The excitation energy of the daughter nucleus was chosen to be  $\Delta_n = 3$  MeV, although this is probably too high a value initially. Our results are not very sensitive to this choice.

In table 2 we show results of the numerical integration, giving  $Y_e$  as a function of  $\rho$ . In deriving phase space factors (eq. (7)) we made approximations. In appendix F the derivation is carried out without these approximations; the  $Y_e$  as function of  $\rho$  which we shall show in table 9 differs only slightly from that obtained from our simple

equation (table 2). In neither of these calculations is neutron drip included and we shall see in appendix F that with its inclusion  $Y_e$  drops appreciably, being  $\sim 0.28$  at  $\rho = 10^{12} \text{ g/cm}^3$  rather than 0.31 found in table 2. It should be remembered that blocking due to some neutrino states being filled, in the density region  $\rho = 10^{11}$  to  $10^{12} \text{ g/cm}^3$  where neutrinos can no longer get out freely (see sect. 4.), has not been taken into account.

#### 4. Neutrino trapping

The neutrino mean free path has been calculated by Lamb and Pethick<sup>16)</sup> to be

$$\lambda_\nu \approx 1.0 \times 10^6 \text{ cm} \left( \frac{\rho}{10^{12} \text{ g/cm}^3} \right)^{-1} \left( \frac{1}{12} X_h \bar{A} + X_n \right)^{-1} \left( \frac{\epsilon_\nu}{10 \text{ MeV}} \right)^{-2}. \quad (16)$$

Here  $X_h$  and  $X_n$  are the mass fractions in heavy nuclei and in neutrons, respectively. This result is based on Weinberg's theory<sup>4)</sup> which gives for the nucleonic neutral current

$$j^\mu = \bar{\psi}_n \frac{\tau_3}{2} \gamma^\mu (1 - \gamma_5) \psi_n - 2 \sin^2 \theta_W \bar{\psi}_n \left( \frac{1 + \tau_3}{2} \right) \gamma^\mu \psi_n, \quad (16.1)$$

where  $\psi_n$  is the nucleon wave function, and  $\theta_W$ , the Weinberg angle. Lamb and Pethick assumed equal numbers of neutrons and protons, and used  $\sin^2 \theta_W = 0.35$ , so the relevant part of  $j_3^\mu$  for them was

$$(j_3^\mu)_{\text{coh}} = -A \sin^2 \theta_W \bar{\psi}_n \gamma^\mu \psi_n = -0.35 A \bar{\psi}_n \gamma^\mu \psi_n. \quad (16.2)$$

In our case, for unequal numbers of neutrons and protons,  $-A \sin^2 \theta_W$  would be replaced by  $-\frac{1}{2}N + \frac{1}{2}(1 - 4 \sin^2 \theta_W)Z$ . On the other hand, the preferred value of  $\sin^2 \theta_W$  is now  $\sim \frac{1}{4}$ , so that, practically, only the first term  $-\frac{1}{2}N = -\frac{1}{2}(1 - Y_e)A$  contributes. For relevant values of  $Y_e \sim 0.30-0.36$ , this is little different from the value  $-0.35A$  used by Lamb and Pethick. More generally, we may replace  $\frac{1}{12}\bar{A}$  in (16) by

$$0.12 \bar{N}, \quad (16.3)$$

where  $\bar{N}$  is the average number of neutrons in the nucleus.

Neutrino trapping begins roughly in Arnett's zone 12 whose physical conditions we listed in eq. (15) ff. Table 1 indicates that for  $Y_e = 0.34$ , the average nucleus has  $A \approx 110$ , hence  $\bar{N} \approx 72$ . Taking  $X_h = 1$ , and substituting (16.3) in (16), we find for  $\epsilon_\nu = 10 \text{ MeV}$ ,

$$\lambda_\nu = 0.85 \times 10^5 \text{ cm}. \quad (16.4)$$

The radius of zone 12 is  $4.27 \times 10^6 \text{ cm}$ , which is about 50 times  $\lambda_\nu$ . Thus we conclude that neutrinos in zone 12 will be effectively trapped.

In appendix C, we calculate the diffusion time for the neutrinos at a density of  $6 \times 10^{12} \text{ g/cm}^3$  and find it to be about 100 msec. The collapse time from  $\rho = 10^{12}$  to  $\rho \approx \infty$ , according to (10), is only 2 msec, so diffusion times are long compared to hydrodynamic ones, indicating effective trapping.

A more precise argument is given in appendix D. Again starting from diffusion theory, we calculate the drift velocity  $v_d$  of neutrinos relative to the nuclear matter; it is directed outward because of the gradient of the neutrino density. This matter moves with a velocity  $u$  relative to the center of the star; we have  $u < 0$  (inward motion). Hence the neutrino radial velocity is

$$\dot{r}_\nu = u + v_d. \quad (16.5)$$

But the core of the star contracts more or less homologously; hence at a given  $r$ , the material density  $\rho$  stays about constant with time. If  $\dot{r}_\nu > 0$ , the neutrinos move (on the average) to lower density and will therefore ultimately escape; if  $\dot{r}_\nu < 0$ , they move with time to higher density and are therefore trapped. The trapping limit,  $\dot{r}_\nu = 0$ , is shown in appendix D to occur at  $\rho < 10^{12}$ .

Once neutrino trapping sets in, the total number of leptons in a given material element remains constant,

$$Y_e + Y_\nu = Y_{et}, \quad (17)$$

where  $Y_{et}$  is the electron fraction at the beginning of trapping. This equation assumes that there is no diffusion of neutrinos, and we show in appendix C that, with the mean free path given by (16), the diffusion is indeed minimal in the short time available ( $< 2$  msec). The lower limit on the outer integral in eq. (7) now becomes  $\mu_\nu$ , so that

$$X = \frac{1}{4} \frac{(\Delta - \mu_\nu)^2 (\Delta^2 + 2\Delta\mu_\nu + 3\mu_\nu^2)}{m_e^2 (k_t^2 / 3m) \mu_e} \quad (17.1)$$

For  $\mu_\nu \rightarrow 0$ , this is identical with (7.2) so there is a smooth transition from the state in which neutrinos flow unimpeded, to the trapping regime. (17.1) may be inserted into (12.6) (which remains unchanged) giving,

$$\frac{d\hat{\mu}}{d\mu_e} = 0.57 \rho_{10}^{1/2} Y_e^2 \frac{\Delta^2 + 2\Delta\mu_\nu + 3\mu_\nu^2}{\mu_e^2} (\Delta - \mu_\nu)^2. \quad (17.2)$$

In the region of trapping  $\mu_\nu$  will increase rapidly as  $\mu_e$  increases and whereas  $\hat{\mu}$  will continue to increase because of some further electron capture,  $d\hat{\mu}/d\mu_e$  will tend to become smaller. Because of the increase in the factors  $\rho_{10}^{1/2}$  and  $(\Delta^2 + 2\Delta\mu_\nu + 3\mu_\nu^2)/\mu_e^2$  in eq. (17.2) and the decrease in  $d\hat{\mu}/d\mu_e$ ,  $\Delta - \mu_\nu$  will quickly become small compared with  $\Delta_n$ , and both quantities will be negligible compared with the  $\mu$ 's. Hence in the trapping region, we soon reach the equilibrium condition

$$\mu_e - \mu_\nu = \hat{\mu} = \mu_n - \mu_p; \quad (18)$$

i.e., the rate of electron capture is fast enough to preserve statistical equilibrium.

The conditions (17) and (18), together with (4), determine  $Y_e$  and  $Y_\nu$  at every density  $\rho$ . Choosing  $\rho = 10^{14}$ , close to nuclear density, and  $Y_{et} = 0.31$ , we get

$$\begin{aligned} Y_\nu &= 0.04, & Y_e &= 0.27, \\ \mu_\nu &= 103, & \mu_e &= 155 \text{ MeV}, \\ \hat{\mu} &= 49 \text{ MeV}, \end{aligned} \quad (18.1)$$

in the trapping region. In this case  $dQ \approx 0$ , and application of eq. (3) gives

$$T(dS)_{\text{per nucleon}} = -dY_e(\mu_e - \hat{\mu} - \mu_\nu) \approx -dY_e \Delta_n, \quad (18.2)$$

since  $\Delta - \mu_\nu$  goes to zero beyond the trapping density, and the excitation energy is approximately equal to the amount the system is out of  $\beta$ -equilibrium. The temperature is now higher,  $> 3$  MeV (see table 4), so the entropy added is only  $0.04 \times \frac{3}{3} = 0.04$  per nucleon. Thus the recognition that neutrinos are trapped<sup>1,2)</sup> was very important for the simple description of the type we give.

### 5. Entropy of nuclei and of nuclear matter

The salient feature in the collapse is the low entropy per nucleon. Drip nucleons would have entropies of 5–10 per nucleon through most of the range of densities covered in the collapse, and the low entropy per nucleon keeps the nucleons mainly inside nuclei. To make quantitative estimates of the proportion of drip nucleons we should estimate the entropy of nucleons inside nuclei. This latter estimate will also tell us the temperature at which nuclear matter is formed when the nuclei squeeze together.

In the Fermi gas model, the nuclear level density at excitation energy  $U$  is given by<sup>17,18)</sup>:

$$\omega(U) = \sum_J (2J+1)\rho(U, J) = \frac{1}{12}\sqrt{\pi} \frac{e^{(4aU)^{1/2}}}{a^{\frac{1}{4}} U^{\frac{3}{4}}}, \quad (19)$$

where  $\rho(U, J)$  is the density of levels of angular momentum  $J$  at energy  $U$ . Here,

$$\frac{a}{A} = \frac{1}{4}\pi^2 \frac{1}{\epsilon_F} \approx 0.067 \text{ MeV}^{-1}. \quad (19.1)$$

We shall use the Fermi gas model as a guide, and later discuss deviations from it.

The partition function  $\Phi$  is obtained from

$$\Phi = \frac{1}{12}\sqrt{\pi}a \int_0^\infty \frac{e^{-U/kT + 2\sqrt{aU}}}{(aU)^{\frac{5}{4}}} dU. \quad (20)$$

Extending the lower limit of the integral to zero would cause difficulties, but it is known that the empirical level density at low excitation energies is substantially less

than that given by eq. (19), so one usually switches over<sup>18)</sup> to an exponential formula, unmodified by the denominator in (19). This switch has the effect of regularizing the integrand at our lower limit. Completing the square,

$$\begin{aligned}\Phi &= \frac{1}{12} \sqrt{\pi} a e^{akT} \int_{-\infty}^{\infty} \frac{e^{-(\sqrt{U/kT} - \sqrt{akT})^2}}{(aU)^{\frac{5}{4}}} dU \\ &= \frac{1}{6} \sqrt{\pi} (akT)^{-\frac{1}{4}} e^{akT} \int_{-\infty}^{\infty} \frac{e^{-(y - \sqrt{akT})^2}}{y^{\frac{3}{2}}} dy.\end{aligned}\quad (20.1)$$

Remembering that the integrand should be changed to something nonsingular for small  $y$ , it is clear that the main contribution to the integral comes from  $y \approx \sqrt{akT}$ . Therefore, we set the  $y^{\frac{3}{2}}$  in the denominator equal to  $(akT)^{\frac{3}{4}}$  and extend the integral from  $-\infty$  to  $\infty$ , obtaining

$$\Phi = \frac{1}{6} \pi \frac{e^{akT}}{akT}. \quad (20.2)$$

This differs slightly from the result of Mazurek *et al.*<sup>19)</sup>, who mistakenly used  $\rho(U, J)$ . (See eq. (19)) rather than  $\omega(u)$ , although their exponential factor was correct. For most of our purposes, the exponential factor  $\exp(akT)$  will be sufficient and, in fact, this is the only reliable part of the expression since the level density at low excitation energies is substantially changed by shell corrections and pairing effects.

Note that the average nuclear excitation energy will be given by the value of  $U$  which makes the exponent in the integrand zero in eq. (20.1), namely,

$$U = a(kT)^2. \quad (20.3)$$

Use of eq. (19.1) gives immediately the excitation energy per particle:

$$\frac{U}{A} = \frac{1}{4} \pi^2 \frac{(kT)^2}{\varepsilon_F}, \quad (20.4)$$

the well-known formula for a degenerate Fermi gas.

The free energy for nuclei is

$$F = -kT \ln \left[ \frac{V}{N} \left( \frac{MkT}{2\pi\hbar^2} \right)^{\frac{3}{2}} \Phi \right], \quad (21)$$

the contribution  $-kT \ln \Phi$  coming from the nuclear level density. As noted, at temperatures  $kT$  of a few MeV the leading term in  $\Phi$  is

$$\Phi \approx e^{akT}. \quad (21.1)$$

The entropy can be obtained from

$$S = -\frac{\partial F}{\partial T}, \quad (21.2)$$

so that the contribution to the entropy from  $\Phi$  of eq. (21) is

$$\frac{S}{k} = \frac{\partial}{\partial T} akT^2 = 2akT. \quad (21.3)$$

Thus, the entropy per nucleon from the level density is

$$\frac{S}{Ak} = \frac{2akT}{A} = \frac{1}{2}\pi^2 \frac{kT}{\epsilon_F}, \quad (21.4)$$

where we have used eq. (19.1). This is the well known entropy per nucleon appropriate for a degenerate Fermi gas of density corresponding to  $k_F = \sqrt{2m\epsilon_F}$ .

The level density parameter  $a$  appropriate for finite nuclei is, however, about twice the theoretical value given by eq. (19.1). A convincing demonstration of this is given in figs. 2-12 of Bohr and Mottelson<sup>20</sup>). Bohr and Mottelson attribute the larger value of  $a$  to the larger effective volume implied by the diffuse surface of the nucleus. It should be noted that the level density also depends upon the effective mass  $m^*$  at the Fermi surface, and the large effective masses found empirically<sup>21</sup>) and explained theoretically<sup>22</sup>) would also tend to increase the level density. In our derivation of the partition function, the low-energy excitations were handled roughly and our derivation is justified only for  $kT$  of the order of a few MeV.

## 6. Equation of state during collapse

In the early stages of the collapse, nuclei partially break up into  $\alpha$ -particles and neutrons<sup>23</sup>). This partial dissolution uses up energy and, therefore, lowers the pressure. This is one of the agencies lowering the effective adiabatic index of the material below  $\frac{4}{3}$ , the other one, in the early stage of the collapse, being the disappearance of leptons through electron capture and the subsequent emission of the neutrinos.

The partial dissolution of nuclei into  $\alpha$ -particles is well understood<sup>23</sup>), although it does not seem to be generally realized that the  $\alpha$ -particles go back into the nuclei at a later stage, a point we shall develop later. In order to bring out quantitatively the relation of this dissolution to entropy, we show in table 3 results for



at a density of  $\rho = 5.9 \times 10^{11} \text{ g/cm}^3$ . The density was chosen because it corresponds to Arnett's zone 13 the last zone before trapping occurs.

Our  $S/k$ , in each case, is the entropy per particle. The total entropy per nucleon is obtained in a straightforward way as

$$\left(\frac{S}{k}\right)_{\text{per nucleon}} = \frac{1}{56} \left[ (1-\delta) \left(\frac{S}{k}\right)_{\text{Fe}} + 13\delta \left(\frac{S}{k}\right)_\alpha + 4\delta \left(\frac{S}{k}\right)_n \right]. \quad (22.1)$$

where  $\delta$  is the fraction of  $^{56}\text{Fe}$  nuclei broken up.

TABLE 3  
Compositions and temperatures for  $\rho = 5.9 \times 10^{11} \text{ g/cm}^3$

(a) Breakup of  $^{56}\text{Fe}$  ( $Y_e = 0.464$ ;  $Q = 124.4 \text{ MeV}$ ).

Proportion $\delta$ of Fe broken up	Entropy per Fe nucleus ( $S/k$ ) <sub>Fe</sub>	Entropy Per $\alpha$ particle ( $S/k$ ) <sub><math>\alpha</math></sub>	Entropy per neutron ( $S/k$ ) <sub>n</sub>	Total entropy per nucleon ( $S/k$ ) <sub>per nucleon</sub>	$kT$ (MeV)
0.1	12.76	8.43	8.22	0.46	1.38
0.2	13.05	7.92	7.71	0.66	1.55
0.3	13.28	7.60	7.39	0.85	1.65
0.4	13.50	7.39	7.18	1.04	1.73
0.5	13.74	7.22	7.01	1.21	1.80
0.6	14.04	7.11	6.90	1.39	1.88

(b) Breakup of  $A_H = 56$  with  $Y_e = 0.393$  ( $Q = 160$ ).

Proportion $\delta$ broken up	Entropy per nucleus	Entropy per $\alpha$ particle	Entropy per neutron	Total entropy per nucleon	$kT$ (MeV)
0.1	12.79	8.62	7.15	0.53	1.41
0.2	13.08	8.11	6.64	0.79	1.58
0.3	13.33	7.81	6.34	1.03	1.70
0.4	13.55	7.60	6.13	1.27	1.79
0.5	13.81	7.45	5.98	1.50	1.88
0.6	14.10	7.33	5.86	1.72	1.96

(c) Breakup of  $A_H = 56$  with  $Y_e = 0.357$  ( $Q = 163$ ) (column headings as given under (b))

0.1	12.73	8.66	6.80	0.55	1.35
0.2	13.03	8.16	6.30	0.84	1.53
0.3	13.28	7.85	6.00	1.10	1.65
0.4	13.51	7.66	5.80	1.35	1.74
0.5	13.77	7.51	5.65	1.60	1.83
0.6	14.06	7.39	5.53	1.84	1.91

\*Entropies in (b) and (c) should be increased, to take into account neutron evaporation from nuclei, before comparison with (a), as discussed in appendix E.

Calculations giving table 3 were carried out using the Saha equation:

$$\frac{n_\alpha^{13} n_n^4}{n_{\text{Fe}}} = \frac{1}{\Phi_{\text{Fe}}} \frac{2^{43}}{(56)^{\frac{3}{2}}} \left( \frac{m k T}{2 \pi \hbar^2} \right)^{24} e^{-Q/kT}, \quad (23)$$

where  $n_{\text{Fe}}$  is the number density for Fe,

$$n_{\text{Fe}} = N_{\text{Fe}} / V, \quad (23.1)$$

$\Phi_{Fe}$  is the partition function,  $n_\alpha$  and  $n_n$  are the number densities for  $\alpha$ -particles and neutrons,  $m$  is the nucleon mass and  $Q = 124.4$  MeV is the  $Q$ -value of the reaction. We assumed  $n_n = \frac{4}{13}n_\alpha$ , corresponding to the dissociation equation (22).

The above calculations are appropriate for  $Y_e = 0.464$ , but as nuclei become neutron rich, major changes occur in their breakup; especially their breakup into  $\alpha$ -particles is strongly inhibited.

In appendix E we discuss a model problem, the breakup of fictitious  $A_H = 56$  nuclei which have  $Y_e = 0.393$  and  $0.357$ , corresponding to 22 and 20 protons, respectively. This allows a direct comparison with the results for  $^{56}\text{Fe}$ , the only difference being the increased neutron richness. The results are given below those for  $^{56}\text{Fe}$  in table 3. From these results, we see that, for a given entropy, there is a smaller amount of breakup, and that the temperature is lower, as compared with the case of  $^{56}\text{Fe}$ , resulting from the larger number of neutrons which carry a higher entropy for the same amount of breakup and temperature.

Although useful for comparison with the  $^{56}\text{Fe}$  breakup, this calculation is unrealistic in at least two aspects: (i) The value of  $A$  will increase with decreasing  $Y_e$ , and this should be taken into account. (ii) Some drip neutrons are present, and these will inhibit the breakup into  $\alpha$ -particles and neutrons (law of mass action). We should, consequently, discuss a three-component system, consisting of nuclei,  $\alpha$ -particles and nucleons. Numerical results will be given in table 10.

Entropies in table 3 for  $Y_e = 0.393$  and  $0.357$  should be increased to take into account neutron drip. For  $Y_e = 0.357$  and  $\delta = 0.1$ , this increase is  $\sim 50\%$ . In the results shown in table 3 we also neglected the nuclear partition function  $\Phi$ . Inclusion of  $\Phi$  according to eq. (21.1) increases the breakup temperature  $kT$  by 0.13 MeV for  $Y_e = 0.357$  and  $\delta = 0.1$ , bringing the results of table 3 close to those of table 10. (For  $Y_e = 0.357$ , the corrected temperature in table 3 for  $\delta = 0.1$  is 1.48 MeV, to be compared with 1.51 MeV for  $\rho = 5.9 \times 10^{11} \text{ g/cm}^3$  from table 10.)

(In appendix E we show that the entropy for  $Y_e = 0.357$  and  $\delta = 0.1$  is about 1.33 per nucleon, to be compared with 1.31 from table 10.)

The relevant Saha equation for the dissociation of  $\alpha$ -particles into nucleons is

$$\frac{n_p^2 n_n^2}{n_\alpha} = 2 \left( \frac{mkT}{2\pi\hbar^2} \right)^{\frac{9}{2}} e^{-Q_\alpha/kT}, \quad (25)$$

where

$$Q_\alpha = 28.3 \text{ MeV}. \quad (25.1)$$

Proton and neutron densities are related by

$$\frac{n_p}{n_n} = e^{(\mu_p - \mu_n)/kT} = e^{-\mu/kT}, \quad (25.2)$$

because  $\mu_p$  and  $\mu_n$  are the same for free nucleons and for those inside nuclei. We see from table 1 that

$$\hat{\mu} = Q_\alpha \quad \text{for } Y_e = 0.315, \quad (25.3)$$

$$2\hat{\mu} = Q_\alpha \quad \text{for } Y_e = 0.378. \quad (25.4)$$

Eq. (25) may now be written as

$$\frac{n_\alpha}{n_n} = \frac{1}{2} \left[ n_n \left( \frac{2\pi\hbar^2}{mkT} \right)^{\frac{3}{2}} \right]^3 e^{(Q_\alpha - 2\hat{\mu})/kT}. \quad (25.5)$$

The expression inside the bracket may be written

$$F = n_n \left( \frac{2\pi\hbar^2}{mkT} \right)^{\frac{3}{2}} = \frac{2.53\rho_{12}X_n}{T^{\frac{3}{2}}} \quad (25.6)$$

where  $T$  is in MeV. For  $X_n \approx 0.1$ ,  $\rho = 10^{13}$  g/cm<sup>3</sup> and  $T \approx 2$  MeV, this is of the order unity. (For lower density or higher temperature, it is even less.) The important factor in (25.5) is, therefore, the exponential, and this is  $\ll 1$  as soon as  $Y_e$  is substantially less than 0.378, eq. (25.4). This is true for most of the interesting region.

When  $Y_e = 0.315$ , eq. (25.3), we even have  $\hat{\mu} = Q_\alpha$  and we may then rewrite (25.5) as

$$\frac{n_\alpha}{n_p} = \frac{1}{2} F^3 e^{(Q_\alpha - \hat{\mu})/kT}. \quad (25.7)$$

Now the exponential is  $\sim 1$ , and thus, if also  $F \approx 1$ ,

$$n_\alpha \approx n_p. \quad (25.8)$$

This means that the  $\alpha$ 's are no more abundant than the very rare protons.

This makes it possible to use the theory of Lattimer and Ravenhall<sup>10)</sup> who have studied the equilibrium between neutron-rich nuclei and a "vapor" consisting of free neutrons and a few protons. This theory takes into account only volume and temperature effects; it leaves out surface, Coulomb and shell effects. The theory is based on a Skyrme interaction between the nucleons; this may somewhat exaggerate the effect of the repulsive core, and thus give too "hard" an equation of state at densities above nuclear density.

The properties of the mixture (including electrons) as a function of density has been calculated by one of us (J.L.) from the Lattimer-Ravenhall theory: The results for  $Y_e = 0.30$  are given in table 4, as a function of the entropy  $S$ , and of the density  $\rho_{13}$  (i.e. in units of  $10^{13}$  g/cm<sup>3</sup>). The temperature is given in MeV, then the percentage of nuclear matter (by mass) which has been evaporated in the form of single nucleons,  $X_n$ . The remainder,  $X_h = 1 - X_n$ , is in heavy nuclei. The next column,  $X_p$ , gives the evaporated protons as a percentage of total nuclear matter. Since the overall fraction of protons is 30%, essentially all of the protons form part of the heavy nuclei. The last column gives the baryon pressure,  $P_b$ , as a percentage of the electron pressure.

TABLE 4

Properties of the equilibrium mixture between neutron-rich nuclei and a free-neutron, free-proton vapor, calculated from the Lattimer-Ravenhall theory for  $Y_e = 0.3$

$S/k$ (per nucleon)	$\rho_{13}$	$T$ (MeV)	$X_n$ (%)	$X_p$ (%)	$P_b/P_e$ (%)
0.5	2.6	2	8	$4 \times 10^{-8}$	3
	10	3	3	$6 \times 10^{-6}$	1.5
	0.33	2	18	$4 \times 10^{-6}$	8
	2.3	4	14	$5 \times 10^{-3}$	8
	4.7	5	11	0.015	7
	9.7	6	7	0.023	5
	0.27	3	24	0.006	20
	2.1	6	21	0.27	17
	5.7	8	15	0.43	15
	9.2	9	10	0.37	11
1.0	0.24	4	30	0.36	32
	2.2	8	28	1.9	28
	4.6	10	24	2.1	24
	8.9	12	16	1.7	20

The value of  $S/k$  includes the electron entropy.

A striking result is the small value of  $X_n$ ; most of the nucleons are in heavy nuclei at all densities up to  $\rho = 10^{14}$ . The reason for the small  $X_n$  is the same as for the small number of  $\alpha$ -particles at  $\rho = 10^{14}$ : the entropy of the heavy nuclei, due to their excitation, is so large that essentially no entropy remains for dissociation – per nucleon, the entropy of the individual nucleons in the vapor is of course still higher. The internal excitation of the heavy nuclei is contained in the Lattimer-Ravenhall theory in the form of the motion of the Fermi gas of nucleons inside the heavy nucleus, precisely the method by which the level-density formula (19) was derived. It should be noted, however, that if we were to use the empirical level density parameter  $a$  in eq. (21.3), which is twice the liquid-drop value used to obtain (21.4) (see the discussion following that equation), we would find an entropy per nucleon of

$$S/k = \pi^2 \frac{kT}{\epsilon_F} \approx 0.25 kT, \quad (25.9)$$

and we would claim that this is the appropriate entropy per nucleon as long as the temperature is high enough to use the approximation (21.1) for  $\Phi$ , if the nuclei are separated. The above does not include the entropy of the electrons, and is, therefore, likely to be an underestimate. From this result (25.9) we see that for entropy  $S/k = 1.5$ ,  $kT$  cannot exceed 6 MeV, which is at variance with the results in table 4. The Lattimer-Ravenhall theory therefore ascribes too little entropy to the nucleus in the nuclei. Part of this is due to leaving out surface effects in their published work <sup>10</sup>).

After completion of that work, these authors found (private communication) that inclusion of entropy from the nuclear surface raised the total entropy per nucleon by  $\sim 50\%$ . This is in line with the discussion of Bohr and Mottelson<sup>20)</sup> who find the level density parameter  $a$  to be increased by 50% in going from the liquid drop model, which has a sharp surface, to the harmonic oscillator potential, which includes surface effects. This increase in  $a$  would be accompanied by the same percentage increase in  $S/k$  (see eq. (21.3)). We can thus understand roughly half the difference between the Lattimer–Ravenhall entropy for nuclei and that implied by eq. (25.9) for the empirical level density parameter. We look to the behavior of the nucleon effective mass in order to explain at least part of the remaining discrepancy. The Skyrme interaction used by Lattimer and Ravenhall<sup>10)</sup> had an effective mass  $m^*/m = 0.9$  while Jeukenne, Lejeune and Mahaux<sup>22)</sup> find that  $m^*$  peaks at larger values ( $\sim 1.2$ ) at an energy somewhat above  $\varepsilon_F$ , just in the region important for us. It is tempting to attribute a substantial part of the large empirical level parameter  $a$ , which is proportional to  $m^*$ , to the peaking of  $m^*$  in this region.

Because of the above considerations, we believe that in the real world, the figures listed under  $S/k = 1.0$  in table 4 would more appropriately refer to a larger entropy,  $S/k \approx 1.5$ , say.

The small fraction of mass in the vapor has the consequence that the nucleons contribute little to the pressure. As long as there is no degeneracy, the pressure is proportional to the number of particles, and that number is clearly small if most of the nucleons are in heavy nuclei. By contrast, in cold neutron-star models such as BBP, most of the nucleons are in the vapor, as free neutrons. The difference in our situation from that in BBP is a direct consequence of our relatively large proportion of protons,  $\sim 30\%$ . Moreover, in this case of BBP the density becomes high enough to lead to degeneracy, which in turn makes for a further increase in pressure. In our case, on the other hand, the pressure is almost entirely due to electrons and neutrinos, as long as the heavy nuclei exist. As long as this is the case, the adiabatic index is close to  $\frac{4}{3}$  and therefore gravitational collapse will continue. This point has been emphasized by Lamb *et al.*<sup>24)</sup> who have shown for reasonable values of the lepton number  $Y_{\text{et}} > 0.2$  and of the entropy  $S/k < 3$ , that in the density interval  $\rho = 10^{13}$  to  $10^{14} \text{ g/cm}^3$  the adiabatic index is less than  $\frac{4}{3}$  because: (a) nucleons are going back into nuclei and (b) the nucleon–nucleon potential is attractive here. The work of these authors shows that the entropy could be double, or the entropy increase three times, what we find here without substantially changing our picture.

For a given density, the fraction evaporated,  $X_n$ , is roughly proportional to the entropy,  $S$ . For given entropy,  $X_n$  decreases with increasing density above  $10^{13} \text{ g/cm}^3$  in accord with table 4. The fraction of evaporated protons is seen to be very small.

The most important result is the pressure due to baryons. This comes from the evaporated nucleons, and since their number is small, the baryon pressure is likewise.

We shall show in the next section that the baryon pressure must be considerably greater than the electron pressure to stop the gravitational collapse. At our low entropy,  $S/k = 1.0$  or  $1.5$ , the baryon pressure is only a small fraction of the electron pressure, and will therefore have hardly any influence on the rate of collapse.

Table 4 and the results of Lamb *et al.*<sup>24)</sup> therefore prove that the collapse cannot be stopped at any density below nuclear density. Once the latter density is reached, the nuclei merge into "one big nucleus" which we may consider as nuclear matter. Inside this, the nucleons move independently and exert pressure, as will be discussed in the next section.

### 7. Densities above nuclear density

At a density somewhat below that of normal nuclear matter, the nuclei will touch, and at about nuclear density  $\rho_0$ , they will merge completely. This transition, for zero temperature, is described in some detail in BBP, sect. 9. Once the nuclei have merged, we have a uniform medium of neutrons and protons to which the Lattimer-Ravenhall theory may be applied.

It was pointed out in the last section that neutrons do not substantially evaporate from nuclei below nuclear density. We see now that above that density, nuclei are squeezed together and change into individual nucleons by squeezing. These nucleons may now be considered as a degenerate Fermi gas with interactions. The interactions are such that at density  $\rho_0 = 0.16$  nucleon per  $\text{fm}^3$  (corresponding to  $2.7 \times 10^{14}$  g/cm<sup>3</sup>) the energy is a minimum, and hence the pressure is zero. Above  $\rho_0$ , the pressure increases rapidly because the kinetic (Fermi) energy dominates over the attractive interaction between the nucleons. The nucleon pressure is *not* due to the hard core in the nuclear interaction (as is sometimes claimed in the literature); the hard core becomes important only at densities of about  $5\rho_0$  or higher.

We calculate the nucleon gas pressure in two ways: (a) by using the empirical compression modulus  $K$  of nuclear matter and (b) from the Lattimer-Ravenhall theory. Finally, we shall use a combination:

(a) The compression modulus is defined as

$$K = 9 dp/d\rho. \quad (26)$$

Recently, it has been possible to determine  $K$  from the energy of the "breathing mode" of heavy nuclei; the result is<sup>25)</sup>

$$K = 220 \text{ MeV}. \quad (26.1)$$

The experiments were done on such nuclei as <sup>208</sup>Pb which has  $Y_e = Z/A = 0.394$ ; we believe that the extrapolation to  $Y_e = 0.36$  or  $0.30$  is justified, especially since  $K$  is not expected to be a sensitive function of  $Y_e$ . The experiment (26.1) refers, of course, to temperature essentially zero, but it is easy to see (cf. table 5) that the pressure does

TABLE 5  
Baryon pressures, Lattimer-Ravenhall, for  $Y_e = 0.36$  and  $Y_e = 0.30$  in MeV/fm<sup>3</sup>

$Y_e = 0.36$		$P_b$		$T(\text{MeV})$	
$\rho(\text{fm}^{-3})$	$S_b = 0.5$	1.0	2.0	$S_b = 1.0$	$S_b = 1.0$
0.16	0.16	0.68	2.78	7.4	0.113
0.20	2.55	3.39	6.76	8.6	0.121
0.24	7.03	8.28	13.3	9.7	0.129
0.32	24.6	26.9	36.5	11.8	0.142
0.40	57.3	61.3	77.2	13.7	0.153
0.48	110	116	140	15.5	0.162

$Y_e = 0.30$		$P_b$		$T(\text{MeV})$	
$\rho(\text{fm}^{-3})$	$S_b = 0.5$	1.0	2.0	$S_b = 1.0$	$S_b = 1.0$
0.16	0.65	1.18	3.26	7.5	0.100
0.20	3.26	4.11	7.45	8.7	0.108
0.24	7.97	9.25	14.2	9.8	0.115
0.32	26.0	28.4	37.8	11.9	0.127
0.40	59.1	63.1	78.9	13.8	0.136
0.48	112	118	142	15.6	0.145

not depend much on temperature (entropy). We shall, in this section, measure pressures in the unit:

$$\text{MeV/fm}^3 = 1.6 \times 10^{33} \text{ dyne/cm}^2. \quad (26.2)$$

In this unit, then, the baryon pressure is

$$p_b = 24.5(\rho - \rho_0), \quad (26.3)$$

where the density is measured in the unit:

$$\text{nucleons/fm}^3 = 1.66 \times 10^{15} \text{ g/cm}^3. \quad (26.4)$$

For  $\rho = 2\rho_0 = 0.32$  nucleons/fm<sup>3</sup>, this gives  $p_b = 3.9$  MeV/fm<sup>3</sup>.

(b) The results of the Lattimer-Ravenhall (LR) theory are given in table 5, for proton fractions  $Y_e = 0.36$  and  $Y_e = 0.30$  and three different values of the entropy in baryons,  $S_b = 0.5, 1$  and  $2$ . The most striking feature is the rapid increase of pressure with density; extrapolating to  $S = 0$ , the data are well fitted by

$$p_b = 2.33[(\rho/\rho_0)^{3.5} - 1]. \quad (27)$$

This is substantially steeper than the result (26.3) derived from constant compres-

sibility; in fact, (27) yields the compression modulus

$$K = 9 \frac{dp_b}{d\rho} = 460 \left( \frac{\rho}{\rho_0} \right)^{2.5}. \quad (27.1)$$

We believe the increase of the compression modulus with density is more realistic than a constant  $K$ ; the increase comes about because the attractive nuclear forces become less important compared to the repulsive forces and the kinetic energy as the density increases. On the other hand, we feel that the empirical  $K = 220$  at  $\rho = \rho_0$  is more accurate than the 460 in (27.1), and we shall therefore multiply the LR pressures by  $\frac{220}{460} = \frac{11}{23}$  in the following calculations. We attribute the excessive compression modulus of 460 to the three-body term in the Skyrme interaction used by LR.

The pressure difference between the different entropies in table 5 is not great. As long as the temperature  $kT$  is small compared with the nucleon Fermi energy  $\epsilon_F$ , the effect on the pressure should be proportional to  $T^2$ , and since  $T$  is proportional to  $S_b$ , according to (21.3), it is also proportional to  $S_b^2$ . Hence we should have at any density,

$$p(S_b = 2) - p(S_b = 1) = 4[p(S_b = 1) - p(S_b = 0.5)]. \quad (27.2)$$

This is well fulfilled in table 5. Finally, the pressure does not appreciably depend on  $Y_e$ , e.g. we find at  $\rho = 0.48$  and  $S = 0.5$ :

$$p(Y_e = 0.3) - p(Y_e = 0.4) = 1.4 \text{ MeV/fm}^3 = 0.025p(Y_e = 0.4). \quad (27.3)$$

In table 5, we also list the temperature for  $S_b = 1$ ; it is in the neighborhood of 10 MeV. (Note that these temperatures are for nuclear matter, not nuclei. See the remarks at the end of sect. 6.) We also give the electron entropy, using (2.2). Both these quantities are proportional to  $S_b$ . The electron entropy adds 11 to 16% to  $S_b$ , so  $S_b = 1$  corresponds to  $S \approx 1.15$ , close to our initial conditions, see sect. 2. (It would have been more useful to calculate the pressures for constant total  $S = S_b + S_e$ , but our procedure saved a lot of work, and the ratio  $S_e/S_b$  is nearly constant in our density range.)

In table 6, we list  $\frac{11}{23}$  of the  $p_b$  calculated for  $S_b = 1$  (in accord with our argument above), to which we add the electron pressure  $p_e$  for the given  $Y_e$  (we assume we have only electrons; if 13% of these are converted into neutrinos, as (18.1) would imply, the combined pressure of the leptons would be slightly smaller for the same total lepton fraction,  $Y_{et}$ ). The total pressure is well represented by

$$p = 3.6(\rho/\rho_0)^{2.5}, \quad (28)$$

although this formula is not quite as accurate as (27) for  $p_b$ . It is also seen that the baryon pressure exceeds the electron pressure above about  $\rho = 0.27$ . The equation (28) corresponds to an adiabatic index

$$\Gamma = 2.5. \quad (28.1)$$

TABLE 6  
Pressures in MeV/fm<sup>3</sup>, for  $S/k = 1$  and  $Y_e = 0.30$

$\rho$ (fm <sup>-3</sup> )	$P_e$	$P_b$	$P$
0.16	2.65	0.56	3.21
0.20	3.57	1.97	5.54
0.24	4.55	4.42	8.97
0.32	6.68	13.6	20.3
0.40	8.99	30.2	39.2
0.48	11.5	56.4	67.9

The energy per nucleon can be calculated by integrating (27) because (27) corresponds to a nucleon adiabat. Multiplying again (27) by  $\frac{11}{23}$ , we get

$$E_b = \int_{\rho_0} p \frac{dp}{\rho^2} = 6.9 \left[ 0.4 \left( \frac{\rho}{\rho_0} \right)^{2.5} + \left( \frac{\rho}{\rho_0} \right)^{-1} - 1.4 \right]. \quad (29)$$

From this we can calculate an approximate value of the density at which the collapse stops, as follows.

If we had the original number of electrons,  $Y_e^{(i)} = 0.42$  per nucleon, then the electron energy would at all times equal the negative gravitational energy; this energy is

$$\begin{aligned} -E_g = E_{e0} &= \frac{3}{4} \mu_e^{(i)} Y_e^{(i)} = \frac{3}{4} 111 (10^{-13} \rho_0 0.42)^{\frac{1}{3}} \left( \frac{\rho}{\rho_0} \right)^{\frac{1}{3}} 0.42 \\ &= 66 (\rho/\rho_0)^{\frac{1}{3}} \text{ MeV/nucleon}. \end{aligned} \quad (29.1)$$

Actually, we have only  $Y_e = 0.31$  electrons per nucleon, so that the electron energy is

$$E_e = (0.31/0.42)^{\frac{1}{3}} E_{e0} = 0.67 E_{e0}. \quad (29.2)$$

In order to stop the inward motion of the material we must have

$$E_b + E_e + E_g = 0, \quad (29.3)$$

and therefore

$$E_b = 22 (\rho/\rho_0)^{\frac{1}{3}}. \quad (29.4)$$

Setting this equal to (29) we find

$$\rho_s/\rho_0 = 2.9 \quad (30)$$

(subscript s for stopping). The inward motion stops only when the density reaches three times normal nuclear density, or  $0.8 \times 10^{15}$  g/cm<sup>3</sup>.

This estimate is very rough. First, we have calculated as if the entire core of the star had the same density; our result can at best apply to some average density, the central

density will be higher, that of the outer part lower. We have neglected, on the one hand, the thermal energy of the nuclear matter, which tends to use up some of the kinetic energy of the collapse. On the other hand, nuclei lose their surface and Coulomb energy upon merging, the transformation of a few of the electrons into neutrinos has lowered the pressure slightly, and the effect of general relativity would be to increase  $|E_g|$ , and therefore to increase the stopping density  $\rho_s$ .

The density  $\rho_s$  is sufficiently high to lead to a pion condensed phase of nuclear matter<sup>26)</sup>;  $\pi^-$  condensation is calculated to occur at twice nuclear matter density<sup>27)</sup> and  $\pi^0$  condensation might appear even earlier, given the large number of protons present. Pion condensation leads to a further softening of the equation of state, so we can foresee reaching densities of  $\sim 10^{15}$  g/cm<sup>3</sup> in the implosion.

The baryon energy increases rapidly near  $\rho_s$ , so the effect is almost as if the material were running into a brick wall. The "bounce" of the stellar material is very hard. We have not investigated the consequences of this on the shock reflected from the center of the star.

In order to get a rough idea on the consequences of this hard bounce, we have applied the Riemann method<sup>28)</sup> to a one-dimensional model for the same equation of state. This indicates that the outer part of the core acquires a substantial outward velocity after it is reached by the shock originating from the "brick wall"; in fact, for a large portion of it, this velocity exceeds the escape velocity (when we translate back to three dimensions). The "hard" equation of state is essential for this result. To obtain quantitative results it will be necessary to do numerical computations in three dimensions, and to treat the outgoing shock caused by the "brick wall" (the Riemann method treats only continuous changes of density and velocity, not shocks). However, on the basis of the one-dimensional model we are very hopeful that the hard equation of state will lead to ejection of material, and thus to the actual supernova phenomenon.

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## Appendix A

### NUCLEAR SYMMETRY ENERGIES

We need, in our work, an expression for  $\hat{\mu} = \mu_n - \mu_p$  which can be used for values of  $Y_e$  smaller than found in known nuclei, and we must be able to determine  $\hat{\mu}$  as a

function of  $A$ , so that a knowledge of individual contributions: bulk, surface and Coulomb, is necessary. Initially, we consider the iron isotopes, because  $^{56}\text{Fe}$  has minimum energy for  $Y_e = 0.464$ . Following eq. (4.5) we can eliminate the Coulomb energy in favor of the surface energy when near a minimum in the energy. In this way we arrived at eq. (4.4).

There is some ambiguity in fitting known masses, in that changes in the bulk symmetry energy can be traded off, to a great extent, against changes in the surface symmetry energy. It is important, therefore, to obtain one or the other independently from the fits to nuclear masses. The bulk symmetry energy is clearly the easier to calculate theoretically. Siemens<sup>29)</sup> obtained a value of 31 MeV for the symmetry energy from the Reid soft core potential, but after correction of an error in his program, this came down<sup>30)</sup> to 27 MeV. This compares well with the value of 28 MeV found, for this potential, by Bäckman<sup>31)</sup>. From the meson-theoretical potential of Jackson, Riska and Verwest<sup>32)</sup>, Bäckman finds 31 MeV. These numbers should be multiplied by 8 to obtain the coefficient in the bulk symmetry energy, and they are then not very far from the 250 MeV in eq. (4.4) taken from BBP.

We rely on Ravenhall, Bennett and Pethick<sup>12)</sup> for the dependence of  $\omega_{\text{surf}}$ , eq. (4.2) on  $Y_e$ .

For  $Y_e \sim \frac{1}{2}$ , we can compare the results of RBP with those of Myers and Swiatecki<sup>33)</sup> who found

$$\omega_{\text{surf}}(Y_e) = \omega_{\text{surf}}(0.5)[1 - (1 - 2Y_e)^2 C_{\text{symm}}]A^{\frac{2}{3}}, \quad (\text{A.1})$$

with  $C_{\text{symm}} = 1.79$  and  $\omega_{\text{surf}}(0.5) = 18.56$  MeV. Expansion of our expression (4.2) about  $Y_e = \frac{1}{2}$  gives  $C_{\text{symm}} = 2.00$ , 10% higher.

Mackie and Baym<sup>34)</sup> arrived at a functional form of the  $Y_e$  dependent surface energy, extrapolating from the situation where the density of drip neutrons is nearly equal to the density inside the nuclei. Expansion of their results about  $Y_e \approx \frac{1}{2}$  gives an expression of the form (A.1) with  $\omega_{\text{surf}}(0.5) = 17.6$  MeV and  $C_{\text{symm}}$  about half the value of Myers and Swiatecki<sup>33)</sup>, even though the value of 27 MeV found by Mackie and Baym for the bulk symmetry energy is close to that obtained by Myers and Swiatecki. Whereas their results for low densities of drip neutrons involves an extrapolation, it is important that they are able to obtain a good fit to the binding energies of medium and heavy ( $A \geq 40$ ) nuclei with their smaller surface symmetry energy.

From fig. 2 of Mackie and Baym, it can be seen that the surface correction to  $\partial W_N / \partial Y_e$ , the quantity determining  $\mu_n - \mu_p$  (see eq. (4)) is substantially smaller than in the results of Ravenhall, Bennett and Pethick<sup>12)</sup>, in the region  $0.3 < Y_e < 0.4$ , so that  $\hat{\mu}$  will be larger, for a given  $Y_e$ . The connection between  $\hat{\mu}$  and  $Y_e$  is particularly used in establishing the  $Y_e$  at neutrino trapping. (See eqs. (15.1) and (15.2).) If we use the expression of Mackie and Baym for the surface energy, we find  $Y_e = 0.33$  at trapping, which is substantially above neutron drip.

Whereas there is ambiguity in the surface symmetry energy, we believe the results of Ravenhall, Bennett and Pethick to give an upper limit for the surface corrections to  $\hat{\mu}$ , or a lower limit for the total  $\hat{\mu}$  in the region  $0.3 < Y_e < 0.4$  important for us.

Let us take  $\omega_{\text{surf}} = 18 \text{ MeV}$ ; there seems to be little ambiguity in this value. We then take the formula:

$$\hat{\mu} = C(0.50 - Y_e) - \frac{\omega_{\text{surf}}}{A^{\frac{1}{3}}} \left\{ \frac{1}{Y_e} + \frac{2}{Y_e} \frac{(1 - 2Y_e)}{(1 - Y_e)} \right\}, \quad (\text{A.2})$$

and determine  $C$  by fits to the known Fe isotopes, masses of which are taken from the Argonne Tables<sup>35</sup>). We find the results shown in table 7. For  $^{52}\text{Fe}$ ,  $Y_e = 0.5$ , and we cannot determine  $C$ . On the other hand, we can then determine  $\omega_{\text{surf}} = 18.0 \text{ MeV}$ , consistent with the value we have assumed.

TABLE 7  
 $\hat{\mu} = \mu_n - \mu_p$  for the Fe isotopes

Isotope <i>A</i>	<i>Y<sub>e</sub></i>	$\hat{\mu} = \mu_n - \mu_p$ from mass tables	Value of <i>C</i> implied by empirical $\hat{\mu}$ (MeV)	$\hat{\mu}$ from Epstein's formula $\mu = 144(0.46 - Y_e)$
50	0.520	-13.97	307	-8.64
52	0.500	-9.66		-5.76
54	0.4815	-4.52	366	-3.10
56	0.464	-0.99	330	-0.58
58	0.448	1.78	305	1.73
60	0.433	4.21	290	3.89

From table 7 it can be seen that the value  $C = 250 \text{ MeV}$  used in the text is, if anything, too small in the region of the Fe isotopes. As discussed above, we believe our surface energy correction to  $\hat{\mu} = \mu_n - \mu_p$  to be too large. Thus, our values of  $\hat{\mu}$  for the  $Y_e$ 's of interest are probably somewhat too small, and we view the value  $Y_e^{(0)} = 0.31$  at trapping to be a lower limit.

## Appendix B

### SHELL-MODEL DESCRIPTION OF ELECTRON CAPTURE

Our discussion in sect. 3 was in terms of the Fermi gas model, although we used an average excitation energy  $\Delta_n$  of 3 MeV for the daughter nucleus which we said would be derived in this appendix. In sect. 3 we found a maximum neutrino energy  $\Delta = 6.9 \text{ MeV}$ . Looking at the derivation there, one finds that protons in the Fermi sea to within a distance of  $\sim \frac{1}{5} \Delta$  will contribute. In the case of the Fermi sea, this means that a fraction

$$f = \frac{1}{5} \Delta \frac{k_f m / \pi^2}{2(\frac{4}{3} \pi k_f^3 / 2\pi)^3} = \frac{3}{5} \frac{\Delta}{k_f^2 / m}, \quad (\text{B.1})$$

will contribute. For  $\Delta = 6.9 \text{ MeV}$ ,  $k_f^2/m = 80 \text{ MeV}$ , a fraction  $f = 0.05$  is implied.

Now in the shell model,  $^{56}\text{Fe}$  has six  $f_{\frac{5}{2}}$  protons, all of which can easily participate. The main Fermi transition to the  $f_{\frac{5}{2}}$  neutron orbitals is blocked, because these are full, but the Gamow-Teller transition to the  $f_{\frac{5}{2}}$  neutron orbital is allowed. The Fermi transition involves  $g_V$ ; the Gamow-Teller  $g_A \sigma \tau_-$ , with  $\tau_- = \sqrt{\frac{1}{2}}(\tau_1 - i\tau_2)$ , and  $g_A \approx 1.25$ . The total transition strength will look like

$$S = g_V^2 \sum (f_{\frac{5}{2}}|1|n)(n|1|f_{\frac{5}{2}}) + g_A^2 \sum (f_{\frac{5}{2}}|\sigma_i \tau_-^*|n)(n|\sigma_i \tau_-|f_{\frac{5}{2}}). \quad (\text{B.2})$$

If all states  $|n\rangle$  were accessible, this sum would be  $S = g_V^2 + 3g_A^2$ , the 3 coming from the three spin orientations, and this sum would be the same as for an initial plane-wave state. As noted,  $|n\rangle = |f_{\frac{5}{2}}\rangle$  is blocked, which cuts out the Fermi transitions and the  $\sim \frac{1}{3}$  of the Gamow-Teller transitions which are not spin flip. Thus, the shell-model ratio to be compared with  $f$  of (B.1) is

$$f_{\text{SM}} \approx \frac{2g_A^2}{g_V^2 + 3g_A^2} \frac{6}{26} = 0.13, \quad (\text{B.3})$$

where  $\frac{6}{26}$  is the ratio of  $f_{\frac{5}{2}}$  protons to total number of protons. Thus, the available strength, because the protons are in the highly favorable  $f_{\frac{5}{2}}$  shell, is 2.6 times that in the Fermi gas model used in sect. 3. Of course, this shell will become partially depleted as the electron capture proceeds, but there will be a general development toward heavier nuclei, which adds some protons.

Note that we have not used the Fermi gas model to estimate the excitation energy of the daughter nucleus; it would give incorrect results. The transitions will be as shown in fig. 1, the  $f_{\frac{5}{2}}$  proton going to the  $f_{\frac{5}{2}}$  neutron orbital. Now, the  $f_{\frac{5}{2}}$  orbital is  $\sim 2 \text{ MeV}$  above the average of  $2p_{\frac{1}{2}}$  and  $2p_{\frac{3}{2}}$  orbitals in  $f_{\frac{5}{2}}$  shell nuclei.

Another effect comes into play. In the capture on  $^{56}\text{Fe}$ , a collective Gamow-Teller state,  $[f_{\frac{5}{2},p}^{-1}, f_{\frac{5}{2},n}]_{T=1}^{1+}$  will be formed. The particle-hole interaction between neutron particle and proton hole is expected to push this state up in energy. Many learned theoretical works have been written about the nuclear forces in this channel, which is also the channel relevant to pion condensation, but here we prefer to look at experiment. In  $^{48}\text{Ca}$ , where all neutron  $f_{\frac{5}{2}}$  levels are filled, the reaction  $^{48}\text{Ca} + ^3\text{He} \rightarrow ^{48}\text{Sc}$  populates preferentially the proton  $f_{\frac{5}{2}}$  and  $f_{\frac{7}{2}}$  states. States ascribed to  $[f_{\frac{5}{2},n}^{-1} f_{\frac{5}{2},p}]^{1+}$  and  $[f_{\frac{5}{2},n}^{-1} f_{\frac{7}{2},p}]^{1+}$  are seen at  $\sim 2$  and  $10 \text{ MeV}$  excitation energy in the final nucleus<sup>36</sup>). The spin-orbit splitting between the  $f_{\frac{5}{2}}$  and  $f_{\frac{7}{2}}$  shells is  $\sim 6 \text{ MeV}$ , so it can be seen that the latter state has been moved up  $\sim 2 \text{ MeV}$  by the particle-hole forces. This

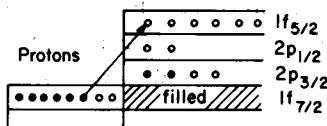


Fig. 1. Shell-model description of the electron capture. In the capture, protons will go to the  $f_{\frac{5}{2}}$  level of the daughter nucleus, which then decays by  $\gamma$ -emission down to the  $2p$  orbitals.

shift involves 8 possible neutron holes times 14 possible proton particles, giving a high degeneracy for the possible particle-hole states. Our initial degeneracy in  $^{56}\text{Fe}$  is 6 proton holes times 6 neutron particles so adding  $\sim 1$  MeV for the collective shift to the  $\sim 2$  MeV for the  $f_{\frac{5}{2}} - 2p$  shell splitting should suffice. In this way we end up at an estimated  $\Delta_n = 3$  MeV.

Had we estimated electron capture rates from nuclear beta decays, and this seems to have been done in most of the literature, we would have obtained much lower rates. Let us consider the  $\beta$ -decay of  $^{49}\text{Ca}$  to  $^{49}\text{Sc}$ , by way of example. The  $J = \frac{3}{2}$  ground state of  $^{49}\text{Ca}$  decays preferably to the  $J = \frac{3}{2}$  excited state of  $^{49}\text{Sc}$ . The shell model would describe both nuclei as  $^{48}\text{Ca}$  plus one  $p_{\frac{3}{2}}$  particle. If the  $\beta$ -decay is then calculated as a single-particle transition of  $p_{\frac{3}{2}}$  neutron to  $p_{\frac{3}{2}}$  proton, the rate is a factor of 30 larger than that found experimentally. Calculation<sup>37)</sup> gives a hindrance factor of 8; this retardation is due to admixture of configurations  $[p_{\frac{3}{2},n}(f_{\frac{5}{2},p}f_{\frac{5}{2},n}^{-1})^{1+}]_{\frac{3}{2}}$  and  $[p_{\frac{3}{2},n}(f_{\frac{5}{2},p}f_{\frac{5}{2},n}^{-1})^{1+}]_{\frac{5}{2}}$ . The admixed configurations are just the components which make up the giant Gamow-Teller collective state. This admixture, through the residual nucleon-nucleon forces, produces a diamagnetism which cuts down strongly matrix elements of  $\sigma$ . Whether one obtains a factor of 8 or of 30 is a delicate matter, since the cancellation is large in either case, and the effective nucleon-nucleon interaction is not known to the necessary accuracy to calculate precisely the small remaining amplitude.

Had we taken the transition  $^{49}\text{Ca} \rightarrow ^{49}\text{Sc}$  to estimate the empirical rate of  $\beta$ -decay and used it in our electron capture calculations, we would have underestimated the rate by a factor of  $\sim 180$  for  $^{56}\text{Fe}$ , a factor of 30 as explained above, and a factor of 6 because all 6  $f_{\frac{5}{2}}$  protons can make the transition to the  $f_{\frac{5}{2}}$  shell-model level in  $^{56}\text{Ca}$ . (The factor of 30 will not be universal, factors of 10 to 100 being typical of the hindrance.)

What we are saying in shell-model language is that ground-state to ground-state or low excited-state transitions are hindered through admixture of the giant Gamow-Teller state, whereas in the electron capture process the transition occurs to the giant Gamow-Teller state itself.

In its role of hindering low-lying  $\beta$ -transitions, the Gamow-Teller state is analogous to the giant dipole state, admixture of which retards low-lying E1 transitions by factors of  $\sim 100$  to 1000. On the other hand, the Gamow-Teller strength has not been found in one relatively concentrated state, as in the case of the giant dipole resonance. This should not matter for the discussion here, since the strength, even if fragmented, should play the same role in hindering low-lying transitions.

In the work of Epstein and Arnett<sup>38)</sup> capture on free protons competed favorably with capture on nuclei, despite the paucity of the former. Whereas the  $X$  relevant for free protons (in this case, just a kinematical factor) is

$$X_{f.p.} = \frac{3}{5} \frac{\mu_e^2}{m_e^2}, \quad (B.4)$$

using (13) and (14) we find the ratio of  $X_{t.p.}$  to the  $X$  for nuclei, eq. (7.2), to be

$$\frac{X_{t.p.}}{X} = 0.99 Y_e^{\frac{3}{2}} \mu_e^{\frac{5}{2}}, \quad (\text{B.5})$$

with  $\mu_e$  in MeV.

For Arnett's<sup>7)</sup> zone 13 ( $\rho = 5.9 \times 10^{11} \text{ g/cm}^3$ ,  $Y_e = 0.356$ ,  $\mu_e = 30.6 \text{ MeV}$ ) in the region just before trapping, this ratio is 1089. From table 10 we see that  $T = 1.51 \text{ MeV}$  for this zone, and from table 1 that  $\hat{\mu} = 19 \text{ MeV}$  for this value of  $Y_e$ ; using (25.2) this gives a ratio

$$n_p/n_n = 2.5 \times 10^{-6}, \quad (\text{B.6})$$

implying  $X_p = 3 \times 10^{-7}$  for  $X_n = 0.1$ . Even with the factor of  $\sim 1000$  retardation found from eq. (B.5), this means that capture on nuclei predominates by a factor of  $3 \times 10^3$  in this zone.

Comparison with table 2 of Mazurek, Truran and Cameron<sup>39)</sup> shows their electron capture rates for nuclei in the region of  $^{56}\text{Fe}$  to be  $\sim 100\text{--}300$  times smaller than ours. Their capture rate on free protons is identical to that given by our eq. (6) (which is slightly larger than that used by Hansen<sup>40)</sup>). Our  $Y_e$ , table 3, are not very different from those of Arnett<sup>7)</sup>, who used the results of Epstein and Arnett<sup>38)</sup> which were based on the rates of Mazurek *et al.*<sup>39)</sup>. This can be understood by the compensation between our large electron capture matrix elements and our large retardation factor arising from the near tracking of  $\mu_e$  by  $\hat{\mu}$ .

Note that our net capture rates and, hence, the  $Y_e$  in table 2 are nearly independent of our input matrix elements. Were we to decrease the numerical factor 2.12 in eq. (8.1) by a factor of 10, then  $\Delta$  as determined by eq. (13.2), would change by a factor of  $(10)^{\frac{1}{4}}$ . This change in  $\Delta$  changes  $X$  in such a way as to compensate for the change in numerical factor, so that the net capture rate does not change much. Such a change in capture rate would, however, change the maximum neutrino energy, which goes as  $\Delta$ .

It should be noted that our low entropy increase in the capture, calculated in sect. 2, does not depend upon the capture proceeding on nuclei, that it would be even lower, were the capture to proceed on free protons. In the latter case, the neutrino is emitted with average energy  $\frac{5}{6} \mu_e$ , a result that follows immediately from phase space arguments and from the fact that the neutron, being heavy, takes up only a negligible part of the electron energy. In terms of our argument, eq. (3) and following, this means that the energy  $\frac{1}{6} \mu_e$  is available for heating the system. On the other hand, as noted in the footnote in sect. 3, free protons used up in the capture have to be replenished from the nuclei, the neutrons formed in electron capture becoming attached to nuclei, and this costs energy  $\hat{\mu} = \mu_n - \mu_p$  per capture, cooling the nuclei. (This is just the familiar process of cooling by evaporation.)

Assuming the neutrinos to escape freely, which they do in the regions of low density where, because of the low temperature, the entropy increase is greatest, this means a net *decrease* in entropy of

$$\left(\frac{\delta S}{k}\right)_{\text{per capture}} = \frac{\frac{1}{6}\mu_e - \hat{\mu}}{kT}. \quad (\text{B.7})$$

(Note also eq. (F.1).) Again for Arnett's zone 13,  $\mu_e = 30.6$  MeV,  $\hat{\mu} = 19$  MeV, and taking a temperature of 1.5 MeV as we did in sect. 2, this gives

$$(\delta S/k)_{\text{per capture}} = -9.3, \quad (\text{B.8})$$

in magnitude more than double the increase in entropy per capture on nuclei, estimated in sect. 2. There is, of course, no reason why the entropy should not decrease, because the system is not closed, with neutrinos escaping. Of course, a decrease in entropy will lower the temperature, shutting the process off since, according to (25.2), the ratio of free protons to free neutrons goes as  $\exp(-\hat{\mu}/kT)$ .

## Appendix C

### DIFFUSION OF NEUTRINOS

The neutrino density  $n_\nu$  is high in the center, and falls off toward the outside. Diffusion may take place, and will be governed by the diffusion equation:

$$\frac{\partial}{\partial t} n_\nu = \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{1}{3} c \lambda_\nu \frac{\partial n_\nu}{\partial r} \right). \quad (\text{C.1})$$

For  $\lambda_\nu$  we use eq. (16); in this we replace  $\varepsilon_\nu$  by  $\mu_\nu$  because effectively only the neutrinos near the top of the Fermi sea can diffuse, and we write:

$$\lambda_\nu = \lambda_0 \left( \frac{\mu_\nu}{10 \text{ MeV}} \right)^{-2}, \quad (\text{C.2})$$

$$\lambda_0 = 1.0 \times 10^6 \text{ cm} \left( \frac{\rho}{10^{12} \text{ g/cm}^3} \right)^{-1} (0.12 X_h \bar{N} + X_n)^{-1}, \quad (\text{C.3})$$

where  $\bar{N}$  is the average number of neutrons in the heavy nucleus. We introduce

$$\mu' = \frac{\mu_\nu}{10 \text{ MeV}}. \quad (\text{C.4})$$

Since  $n_\nu$  is proportional to  $\mu_\nu^3$ , we replace it by  $\mu'^3$  in (C.1) and have,

$$\frac{\partial}{\partial t} (\mu'^3) = \frac{1}{3r^2} \frac{\partial}{\partial r} \left( r^2 c \lambda_0 \mu'^{-2} \frac{\partial}{\partial r} (\mu'^3) \right). \quad (\text{C.5})$$

We shall consider  $\lambda_0$  as constant, although in reality  $\rho$ , the matter density, varies with  $r$ . Then:

$$\mu'^2 \frac{\partial \mu'}{\partial t} = \frac{1}{3} c \lambda_0 \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial \mu'}{\partial r} \right). \quad (\text{C.6})$$

A particular solution can be obtained by separation of variables; write:

$$\mu' = \mu'_0 \psi(r) \phi(t) \quad (\text{C.7})$$

Then (C.6) becomes

$$\psi^3 \phi^2 \frac{d\phi}{dt} = \frac{c \lambda_0}{3 \mu_0'^2} \frac{\phi}{r^2} \frac{d}{dr} \left( r^2 \frac{d\psi}{dr} \right) \quad (\text{C.8})$$

We divide by  $\psi^3 \phi$  and set each side of the equation equal to a separation constant which we call  $-\frac{1}{2}a$ , thus:

$$\frac{\phi}{dt} \frac{d\phi}{dt} = -\frac{1}{2}a, \quad (\text{C.9})$$

$$\frac{1}{r^2} \frac{d}{dr} \left( r^2 \frac{d\psi}{dr} \right) = -\frac{3 \mu_0'^2 a}{2 \lambda_0 c} \psi^3. \quad (\text{C.10})$$

(C.9) has the solution,

$$\phi = (1 - at)^{\frac{1}{2}}. \quad (\text{C.11})$$

(C.10) is of the type of the Lane-Emden equation of a polytrope. We define:

$$x = \left( \frac{3 \mu_0'^2 a}{2 \lambda_0 c} \right)^{\frac{1}{2}} r, \quad (\text{C.12})$$

and obtain,

$$\frac{1}{x^2} \frac{d}{dx} \left( x^2 \frac{d\psi}{dx} \right) = -\psi^3. \quad (\text{C.13})$$

This is the Lane-Emden equation<sup>41)</sup> of index 3 whose solution is known. The separation constant is determined by the condition that  $\mu_r$  (and hence  $\psi$ ) must be 0 at some radius  $R$ , i.e. the radius at which neutrino trapping occurs. The zero of the Lane-Emden function of order 3 is at  $x = 6.9$ ; hence from (C.12):

$$a = \frac{2 \lambda_0 c}{3 \mu_0'^2} \left( \frac{6.9}{R} \right)^2. \quad (\text{C.14})$$

For the Lane-Emden equation of order 3, the ratio of the central to the average density is,

$$\frac{n_c}{n_{Av}} = \left( \frac{\mu_0}{\mu_{Av}} \right)^3 = 54.2, \quad (\text{C.15})$$

i.e. there is strong central condensation.

Typical values <sup>7)</sup>, relating to the middle of the region of trapped neutrinos (Arnett's mass point 9) are†:

$$\rho = 5.9 \times 10^{12}, \quad R = 3.2 \times 10^6, \quad \mu_\nu = 35 \text{ MeV}, \quad \bar{N} = 85. \quad (\text{C.16})$$

We take this value of 35 MeV to be  $\mu_{Av}$ ; then (C.15) gives

$$\mu_0 = 133 \text{ MeV}, \quad \mu'_0 = 13.3. \quad (\text{C.17})$$

This is close to the central  $\mu_\nu$  we calculated in (18.1). Inserting in (C.3), we find  $\lambda_0 = 1.7 \times 10^4 \text{ cm}$ , and

$$a = 9 \text{ sec}^{-1}. \quad (\text{C.18})$$

So it takes about  $\frac{1}{9}$  sec for the neutrinos to get out of the material. This is many times longer than the time scale of the hydrodynamics, cf. eq. (10). This shows that the neutrino diffusion, in the bulk of the core, is negligible during the times relevant to the hydrodynamics, as stated at the end of sect. 3. It may be noted that  $\lambda_0/R^2$  in (C.14) is proportional to  $1/\rho R^2$  which is not strongly dependent on  $\rho$ , thus the time scale (C.18) will not change much if the star is further compressed or expanded.

It is likely that the radial distribution of  $\mu_\nu$  is not as peaked at the center as the Lane-Emden function,  $\psi$ , eq. (C.13). In this case, (C.6) makes it likely that  $\mu'$  decreases fastest with time where  $\mu'$  is small, i.e. near the surface of the region of trapped neutrinos. Therefore we may expect that this surface gradually moves inward, relative to the matter; there is a "neutrino rarefaction wave" moving inward. This result has also been obtained by Lichtenstein *et al.*<sup>13)</sup>.

## Appendix D

### TRAPPING CRITERION

The diffusion theory which we discussed in appendix C gives an expression for the radial current of neutrinos,

$$S = -\frac{1}{3}c\lambda_\nu \frac{\partial n_\nu}{\partial r}. \quad (\text{D.1})$$

We use (C.2) for  $\lambda_\nu$  and set

$$n_\nu = K\mu_\nu^3, \quad K = \frac{1}{6\pi^2(\hbar c)^3}. \quad (\text{D.2})$$

then

$$S = -100c\lambda_0 K \frac{\partial \mu_\nu}{\partial r}. \quad (\text{D.3})$$

† For  $R$ , we have chosen  $2^{\frac{1}{3}}$  times the radius of mass point 9, which would be the radius of the trapped-neutrino sphere if the density were constant at the value in zone 9.

We may define a drift velocity of the neutrinos

$$v_d = \frac{S}{n_\nu}; \quad (D.4)$$

it gives the average velocity of the neutrinos relative to the nuclear material which does the scattering;  $v_d$  is positive which indicates a relative motion outward. Inserting (D.3), (D.2), (C.2),

$$v_d = -100 \frac{c\lambda_1}{\rho_{12}\mu_\nu^3} \frac{\partial\mu_\nu}{\partial r}, \quad (D.5)$$

where  $\lambda_1$  is the value of  $\lambda_0$ , (C.3), for  $\rho = 10^{12}$ , and  $\rho_{12}$  the density in units of  $10^{12}$  g/cm<sup>3</sup>; with  $X_h = 1$ ,  $\bar{N} = 72$ , we have

$$\lambda_1 = 1.15 \text{ km.} \quad (D.6)$$

Table 8 gives the relevant quantities in (D.5), using Arnett's Tables I and II. It is possible that the values of  $\mu_\nu$  should actually be somewhat lower than those given by Arnett because Arnett obtains too low values for  $Y_e$  for high densities (as compared to ours), indicating that he assumes too much transformation of electrons into neutrinos and therefore too high a neutrino density. However, Arnett's is the best calculation available, and his numbers should at least indicate the trend.

TABLE 8  
Neutrino drift velocity

Zone* $k$	$-\partial\mu_\nu/\partial r$ (MeV/km)	$\rho_{12}$	$(\mu_\nu/10)^3$ (MeV)	$v_d$ ( $10^8$ cm/sec)	$-u_k$ ( $10^8$ cm/sec)
8	1.15	7.9	61	0.08	5.9
9	1.25	5.9	43	0.17	7.4
10	1.02	3.6	24	0.41	9.8
11	1.17	2.25	11	1.66	12.5
12	0.82	1.35	4.9	4.3	15.2
13	0.35	0.59	1.73	11.9	18.2
14	0.162	0.214	0.50	52	20.2

\* Arnett denotes by  $k$  the zone between his mass points  $k-1$  and  $k$ .

$v_d$  is the neutrino drift velocity,  $u_k$  the material velocity.

Table 8 shows that  $\partial\mu_\nu/\partial r$  is nearly constant up to zone 11, then drops fairly rapidly. Both  $\rho_{12}$  and  $\mu_\nu^3 \approx n_\nu$  decrease rapidly toward the outside. Therefore, the drift velocity  $v_d$ , calculated from (D.5), increases very rapidly with zone number  $k$  (for  $k = 14$ , the diffusion theory underlying (D.5) may no longer be valid). The

velocity of the nuclear matter,  $u_k$ , changes only slowly by comparison. Therefore, the net velocity of the neutrinos relative to the star center,

$$\dot{r}_\nu = u + v_d, \quad (16.5)$$

goes through zero with a big slope. The point  $\dot{r}_\nu = 0$  can thus be determined with high accuracy; it lies between zones 13 and 14, at a density

$$\rho_{12} \approx 0.43. \quad (D.7)$$

If Arnett's values for  $\mu_\nu$  are decreased, as proposed above,  $v_d$  will be increased, and hence the point  $\dot{r}_\nu = 0$  will be shifted to somewhat higher density, but we do not believe that this shift can be as much as a full zone. Thus we think it is safe to say that the critical density for trapping,

$$\rho_{\text{trap}} < 10^{12} \text{ g/cm}^3. \quad (D.8)$$

## Appendix E

### DISSOCIATION OF NEUTRON-RICH NUCLEI

In order to see how neutron richness affects the breakup of nuclei, we discuss fictitious  $A_H = 56$  nuclei, with  $Y_e = 0.393$  and  $Y_e = 0.357$ , corresponding to 22 and 20 protons, respectively. We take  $\rho = 5.9 \times 10^{11} \text{ g/cm}^3$  so that we can compare with the  $^{56}\text{Fe}$  breakup, top of table 3.

In order to calculate the  $Q$ -value for the breakup, we must calculate the lowering of the binding energies of our  $A_H = 56$  nuclei with  $Y_e = 0.393$  and  $Y_e = 0.357$  relative to that of  $^{56}\text{Fe}$ . We use Epstein's formula (4.3) obtained from empirical binding energies in this region of  $A$ .

The binding energy of the  $A = 56$  nucleus is then lowered by

$$\delta E = 56 (0.46 - Y_e)^2 \frac{1}{2}(144 \text{ MeV}). \quad (E.1)$$

We have approximated here the  $Y_e = 0.464$  appropriate for  $^{56}\text{Fe}$  by 0.46. On the other hand, there will be a decrease in the number of  $\alpha$ -particles in the breakup and, therefore, a decrease in the binding energy of the dissociated particles of

$$\delta E_\alpha = \frac{56}{2}(0.46 - Y_e) 28.3 \text{ MeV}. \quad (E.2)$$

This leads to an increase in  $Q$ -value for the breakup of

$$\delta Q = \delta E_\alpha - \delta E = \frac{56}{2} [28.3 - (0.46 - Y_e)144 \text{ MeV}](0.46 - Y_e). \quad (E.3)$$

For  $Y_e = 0.393$ ,  $\delta Q \approx 35 \text{ MeV}$ , so that our  $Q$ -value is

$$Q = 124 + 35 = 159 \text{ MeV}, \quad (E.4)$$

and for  $Y_e = 0.357$ ,

$$Q = 163 \text{ MeV.} \quad (\text{E.5})$$

We next carried out calculations using eq. (23), appropriately changed for 11  $\alpha$ -particles and 12 neutrons for the case of  $Y_e = 0.393$  and for 10  $\alpha$ -particles and 16 neutrons for  $Y_e = 0.357$ . The results are given in the lower part of table 3. These entropies should be increased  $\sim 50\%$  because of neutron evaporation from nuclei



according to

$$\frac{n_{A-1}n_n}{n_A} = \frac{\Phi_{A-1}}{\Phi_A} 2 \left( \frac{mkT}{2\pi\hbar^2} \right)^{\frac{3}{2}} e^{-Q_n/kT}, \quad (\text{E.6})$$

where  $Q_n$  is the neutron binding energy,  $\geq 5$  MeV in these neutron rich nuclei with  $Y_e = 0.35-0.40$ . There will be many atomic species in the medium, but their abundance will clearly have a maximum at some value of  $Z$  and  $A$ . Near that maximum,  $n_{A-1} = n_A$ ; assuming then also  $\Phi_{A-1} = \Phi_A$ , we can easily calculate  $X_n$  from (E.6).

To this entropy due to nuclear breakup we should add two terms which we calculate for  $\delta = 0.1$  and  $Y_e = 0.393$  and 0.357, hence for temperatures of 1.40 and 1.35 MeV (see table 3). They are: (a) the entropy due to the excitation of the nuclei, using (25.9) which gives 0.35 or 0.34, respectively, and (b) the entropy in the electrons, 0.17 or 0.16; thus, we end up with a total entropy of 1.32 or 1.33, just about right. Our temperatures of 1.40 and 1.35 MeV are substantially lower than Arnett's 1.90 MeV for this density; we shall come back to a discussion of this later.

From our results in table 3 for the entropy in translational motion, we see that for a given  $\delta$ , the entropy is increased as  $Y_e$  is lowered. Thus, for a given entropy,  $\delta$  must be lowered. The entropy increase comes from the larger number of neutrons in the breakup. Already when  $Y_e$  has decreased to 0.393 we see relatively little breakup with  $\alpha$ -particles ( $\delta \approx 0.1$  as compared with  $\delta \approx 0.2$  for  $^{56}\text{Fe}$ ).

Arnett<sup>7</sup>), with  $X_h = 0.57$ ,  $X_n = 0.10$  and  $X_\alpha = 0.33$  and  $kT = 1.90$  MeV for  $\rho = 5.9 \times 10^{11} \text{ g/cm}^3$  has a greater breakup, substantially more  $\alpha$ -particles and a higher temperature. Arnett neglected the entropy from the level density in nuclei; had he included it, less entropy would have been in translational motion and his temperature would have been lower, although still somewhat above ours. Our eqs. (25.5) and (25.6) show that Arnett's effective  $\hat{\mu}$  was  $\sim 7$  MeV, much too small for his  $Y_e = 0.356$  where 19 MeV would be more appropriate.

From our model calculations in this appendix, we see then how the increased number of neutrons in the breakup of neutron-rich nuclei inhibits, for a given entropy, that breakup. Even if  $Y_e$  remained at 0.464, the value appropriate for  $^{56}\text{Fe}$ ,  $\alpha$ -particles would tend to go back into nuclei with increasing density  $\rho$ . Our considerations here show this tendency to be much more pronounced for smaller values of  $Y_e$ . The role of the  $\alpha$ -particle is very minor.

### Appendix F

ELECTRON NUMBERS, ENTROPIES AND TEMPERATURES, AS FUNCTIONS OF DENSITY  $\rho$ .

In this appendix we present results of an explicit integration of eq. (11). To determine also the temperature, we use the first law of thermodynamics to follow the entropy change,

$$T \left( \frac{dS}{d \ln \rho} \right)_{\text{per nucleon}} = - \frac{d Y_e}{d \ln \rho} (\mu_e - \mu_n + \mu_p - 1.297 - \bar{\epsilon}_\nu), \quad (\text{F.1})$$

where 1.297 is the neutron-proton mass difference and  $\bar{\epsilon}_\nu$  is the average energy of the neutrino created in electron capture. This equation is valid only when the matter is completely transparent to neutrinos. Instead of using eq. (17.2) for  $X$  in eq. (11), eq. (7) has been integrated without the assumption that  $\epsilon_e = \mu_e$ , but rather that

$$\epsilon_e = \epsilon_\nu + \hat{\mu} + \Delta_n + \Delta_p + 1.297. \quad (\text{F.2})$$

Thus, we use here

$$X = \frac{1}{6} \frac{(\mu_e - Q)^4}{m_e^2 (k_f^2 / 3m) \mu_e} \left( 1 + \frac{2}{5} \frac{Q}{\mu_e} + \frac{1}{10} \frac{Q^2}{\mu_e^2} \right), \quad (\text{F.3})$$

where  $Q = \hat{\mu} + \Delta_n + 1.297$ . To find  $\bar{\epsilon}_\nu$ , we replace  $\epsilon_\nu^2$  in eq. (7) by  $\epsilon_\nu^3$  and call the integral  $Y$ :

$$Y = \frac{3}{28} \frac{(\mu_e - Q)^5}{m_e^2 (k_f^2 / 3m) \mu_e} \left( 1 + \frac{1}{3} \frac{Q}{\mu_e} + \frac{1}{15} \frac{Q^2}{\mu_e^2} \right). \quad (\text{F.4})$$

Then,

$$\bar{\epsilon}_\nu = \frac{Y}{X}. \quad (\text{F.5})$$

As  $\hat{\mu}$  follows  $\mu_e$  more and more closely, one then finds that  $\bar{\epsilon}_\nu \approx \frac{3}{5}(\mu_e - Q)$ , but we do not assume this here.

Eqs. (11) and (F.1) have been integrated from the initial conditions  $\rho = 3.7 \times 10^9 \text{ g/cm}^3$ ,  $Y_e = 0.42$  and  $T = 0.69 \text{ MeV}$  up to  $\rho = 10^{12} \text{ g/cm}^3$ , using  $\Delta_n = 3 \text{ MeV}$ . We first consider the case in which dripped neutrons are neglected. The entropy per nucleon  $S$  is the sum of electron (eq.(2.2)), nuclear translational (eq. (2)) and internal nuclear (eq. (25.9)) terms. Results are given in table 9.

We see for conditions near Arnett's zone 12,  $\rho = 1.35 \times 10^{12} \text{ g/cm}^3$  that  $Y_e \approx 0.32$ . This is slightly higher than the  $Y_e^{(t)} = 0.31$  derived in eq. (15.2) and given in table 2 because the righthand side of eq. (F.3) is always less than that of eq. (7.2). Also, the temperature is quite high near  $10^{12} \text{ gm/cm}^3$  because the entropy of dripped neutrons has been neglected. In turn, the entropy generation is too small because of the high temperature.

TABLE 9  
Electron numbers, temperatures and entropies, calculated without inclusion of neutron drip

$\rho_{10}$	$Y_e$	$T(\text{MeV})$	$S/k$	$\hat{\mu}(\text{MeV})$	$\mu_e(\text{MeV})$	$\Delta(\text{MeV})$
0.37	0.420	0.69	0.905	4.38	5.96	
0.50	0.420	0.75	0.905	4.42	6.59	
0.67	0.420	0.81	0.905	4.44	7.28	
0.91	0.420	0.87	0.905	4.47	8.04	
1.22	0.420	0.93	0.905	4.49	8.88	0.09
1.65	0.420	1.00	0.905	4.53	9.81	0.99
2.22	0.420	1.07	0.905	4.57	10.83	1.97
2.99	0.420	1.15	0.906	4.65	11.97	3.03
4.03	0.419	1.23	0.909	4.86	13.21	4.06
5.43	0.417	1.33	0.918	5.35	14.56	4.92
7.32	0.412	1.45	0.933	6.23	16.03	5.51
9.87	0.406	1.59	0.954	7.48	17.62	5.84
13.30	0.399	1.74	0.977	9.03	19.35	6.02
17.93	0.391	1.91	1.002	10.79	21.22	6.13
24.16	0.382	2.08	1.026	12.75	23.26	6.21
32.57	0.372	2.26	1.051	14.88	25.47	6.29
43.90	0.362	2.45	1.075	17.21	27.88	6.37
59.17	0.351	2.64	1.098	19.73	30.48	6.45
79.75	0.339	2.83	1.122	22.46	33.29	6.53
107.5	0.327	3.02	1.145	25.40	36.33	6.63
131.2	0.318	3.16	1.160	27.49	38.49	6.70

Entropy is given as entropy per nucleon.

We now wish to investigate the effects of neutron drip on these results. Eqs. (11) and (F.1)–(F.5) are still valid, as is eq. (14.1) for  $\mu_e$ , but eq. (4.4) for  $\hat{\mu}$ , eq. (5) for  $A$  and eq. (5.3) for  $\mu_n$  must be modified by replacing  $Y_e$  in them by  $x = Z/A$ , related to  $Y_e$  by

$$x = Y_e / (1 - X_n). \quad (\text{F.5.1})$$

Since the drip neutrons are essentially free in the density range of interest, one can make use of eq. (25.6) to find  $X_n$ :

$$X_n = \frac{n_n}{\rho} = 79 \frac{T^{\frac{3}{2}}}{\rho_{10}} e^{\mu_n/T}, \quad (\text{F.6})$$

with  $T$  measured in MeV. Alpha particles were included, but they turn out to be negligible throughout these calculations (see eq. (25.5)). Nuclear entropy was included according to eq. (25.9). The entropy of dripped neutrons is included using a formula similar to that for nuclei, eq. (2):

$$\left(\frac{S}{k}\right)_{\text{per dripped nucleon}} = \frac{5}{2} + \ln \left[ \frac{2V}{N_n} \left( \frac{mkT}{2\pi\hbar^2} \right)^{\frac{3}{2}} \right]. \quad (\text{F.6.1})$$

TABLE 10  
Electron numbers, temperatures and entropies, calculated with neutron drip

$\rho_{10}$	$Y_e$	$T(\text{MeV})$	$X_n$	$S/k$	$\hat{\mu}(\text{MeV})$	$\mu_n(\text{MeV})$	$\Delta(\text{MeV})$
0.37	0.420	0.69	1.7(-4)	0.905	4.38	-9.30	
0.50	0.420	0.74	3.6(-4)	0.905	4.39	-9.30	
0.67	0.420	0.80	6.9(-4)	0.905	4.39	-9.31	
0.91	0.420	0.85	1.21(-3)	0.905	4.37	-9.32	
1.22	0.420	0.90	1.81(-3)	0.905	4.35	-9.34	0.23
1.65	0.420	0.96	2.5(-3)	0.905	4.33	-9.36	1.18
2.22	0.420	1.01	3.4(-3)	0.905	4.31	-9.37	2.22
2.99	0.420	1.07	4.4(-3)	0.906	4.35	-9.37	3.32
4.03	0.418	1.12	5.9(-3)	0.910	4.54	-9.30	4.37
5.43	0.415	1.18	8.7(-3)	0.922	5.01	-9.11	5.23
7.32	0.409	1.24	0.0127	0.943	5.84	-8.77	5.86
9.87	0.401	1.30	0.0192	0.973	6.98	-8.31	6.27
13.30	0.391	1.34	0.0283	1.012	8.36	-7.77	6.56
17.93	0.379	1.38	0.0402	1.057	9.92	-7.16	6.80
24.16	0.366	1.42	0.0553	1.109	11.61	-6.52	7.02
32.57	0.351	1.45	0.0742	1.167	13.43	-5.84	7.25
43.90	0.334	1.47	0.0978	1.233	15.35	-5.15	7.50
59.17	0.315	1.51	0.127	1.307	17.33	-4.46	7.79
79.75	0.295	1.54	0.165	1.390	19.34	-3.77	8.13
107.5	0.271	1.60	0.211	1.481	21.33	-3.12	8.52
131.2	0.255	1.65	0.248	1.547	22.61	-2.71	8.82

Entropy is given as entropy per nucleon.

The integrations including neutron drip are displayed in table 10. At  $\rho = 10^{12} \text{ g/cm}^3$ ,  $Y_e^{(0)} \approx 0.28$ , so that the effect of drip neutrons is small, even though  $X_n \approx 0.2$  here. The partial dissociations of nuclei acts as a thermostat to keep the temperature low. Because  $x > Y_e$ ,  $\hat{\mu}$  is less in this case and neutrino energy is higher in table 10 than in table 9. As a result, the entropy generation is more than doubled. Even so, the entropy does not exceed  $\approx 1.5$  per nucleon, in agreement with our earlier discussion.

In the above calculation of entropy production we have neglected contributions from downscattering in energy of the emitted neutrinos. As noted above, the average neutrino energy is  $\bar{\epsilon}_\nu = \frac{3}{5}\Delta$  so that a downscattered neutrino which deposits all of its energy in the system would increase the entropy by

$$\delta S = \bar{\epsilon}_\nu/kT = \frac{3}{5}\Delta/kT. \quad (\text{F.7})$$

Neutrinos elastically scattered from nuclei will deposit only recoil energy

$$E_R \approx \epsilon_\nu^2/2Am, \quad (\text{F.8})$$

where  $m$  is the nucleon mass, and this is negligibly small. Down-scattering in energy will proceed only through neutrino-electron scattering.

For the ratio of mean free paths for scattering off electrons to coherent scattering off nuclei we find

$$\frac{\lambda_e}{\lambda_{el}} = \frac{2}{Y_e} \left[ \frac{\bar{N}^2}{6A} X_h + X_n \right] \frac{\mu_e}{\varepsilon_\nu}, \quad (\text{F.9})$$

from eq. (14) of Lamb and Pethick<sup>16</sup>), with replacement through our eq. (16.3). The final factor ( $\mu_e/\varepsilon_\nu$ ) results from electron degeneracy. For Arnett's zone 12, this ratio is

$$\frac{\lambda_e}{\lambda_{el}} \approx 640, \quad (\text{F.10})$$

where we have used  $\bar{N} = 88$ ,  $\varepsilon_\nu = \bar{\varepsilon}_\nu = 4.15$  MeV,  $\mu_e = 39.1$  MeV,  $Y_e = 0.31$ . Since, as found earlier,  $\lambda_{el}/R \approx \frac{1}{10}$ , where  $R = 4.27 \times 10^6$  cm is the radius of this zone, the probability of neutrino-electron downscattering at this density looks small.

The possible importance of neutrino downscattering in increasing the entropy was pointed out to us by Don Lamb, and we would like to thank him for extensive discussions.

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**Equation of State of a Very Hot Gas of  
Electrons and Neutrinos**  
(with J. H. Applegate and G. E. Brown)  
*Astrophys. J.* **241**, 350–354 (1980)

Published as an appendix to the paper “Neutrino Emission from a Supernova Shock”, this is a useful collection of formulae for the treatment of supernova shocks. The temperature is assumed to be  $kT \geq \frac{1}{4}$  MeV, so that electrons are fully relativistic.

## APPENDIX

The equation of state of an ideal gas of electrons, positrons, electron neutrinos, and electron antineutrinos in beta equilibrium with an ideal gas of nucleons has been worked out by Van Riper and Bludman (1977). The relativistic particles are in thermal and chemical equilibrium with blackbody photons. We give details of the calculation here and a table of the equation of state. The blackbody photons may produce electron-positron pairs directly. All types of neutrino-antineutrino pairs may be produced by the electron-positron gas by coupling through the weak neutral current, as pictured in Figure 1.

The neutrino-antineutrino pairs produced in thermal equilibrium by the process pictured in Figure 1 will be distributed in energy as blackbody radiation (i.e., with zero chemical potential) as long as no excess of particles over antiparticles exists. The  $\mu$  and  $\tau$  neutrinos in the stellar material are all produced by pair production; hence they are present in equal numbers and are distributed in energy as blackbody radiation. Electron neutrinos and antineutrinos may be present in different numbers because of the trapping of electron neutrinos during the infall of the core, and because they are created and destroyed in maintaining beta equilibrium with the nucleons. Because the  $\mu$  and  $\tau$  neutrinos are always blackbody, they need not be treated in this equation of state.

The particle densities and energy densities of the relativistic particles are given in terms of the temperature (measured in energy units; Boltzmann's constant is equal to unity) and chemical potentials by equation (A1) for electrons and positrons, and equation (A2) for neutrinos and antineutrinos:

$$n_{e^{\pm}} = \frac{1}{\pi^2} \left( \frac{T}{\hbar c} \right)^3 F_2 \left( \frac{\mu_{e^{\pm}}}{T} \right), \quad e_{e^{\pm}} = \frac{T}{\pi^2} \left( \frac{T}{\hbar c} \right)^3 F_3 \left( \frac{\mu_{e^{\pm}}}{T} \right); \quad (A1)$$

$$n_{\nu_e, \bar{\nu}_e} = \frac{1}{2\pi^2} \left( \frac{T}{\hbar c} \right)^3 F_2 \left( \frac{\mu_{\nu_e, \bar{\nu}_e}}{T} \right), \quad e_{\nu_e, \bar{\nu}_e} = \frac{T}{2\pi^2} \left( \frac{T}{\hbar c} \right)^3 F_3 \left( \frac{\mu_{\nu_e, \bar{\nu}_e}}{T} \right). \quad (A2)$$

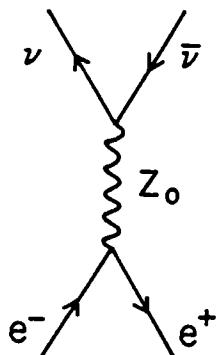


FIG. 1.—Neutrino pair production by the electron-positron gas

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The functions  $F_2(x)$  and  $F_3(x)$  are the Fermi integrals

$$F_2(x) = \int_0^\infty \frac{t^2}{1 + e^{(t-x)}} dt, \quad F_3(x) = \int_0^\infty \frac{t^3}{1 + e^{(t-x)}} dt. \quad (\text{A3})$$

The factor of 2 difference between the  $e^+e^-$  gas formulae (A1) and the  $\bar{\nu}\bar{\nu}$  gas formulae (A2) comes from the electron spin degeneracy (two spin states) as opposed to the neutrino spin degeneracy (one helicity state). In deriving (A1), the electron rest mass has been ignored.

The electron-positron gas and the neutrino-antineutrino gas are in equilibrium with the radiation field. Thus, the sum of particle and antiparticle chemical potential must be zero:

$$\mu_{e^-} + \mu_{e^+} = \mu_{\text{photon}} = 0, \quad \mu_{\nu_e} + \mu_{\bar{\nu}_e} = \mu_{\text{photon}} = 0. \quad (\text{A4})$$

The number densities of electrons and positrons are related to the number density of protons by the charge neutrality of the stellar material:

$$n_p = Y_p n_B = n_{e^-} - n_{e^+}. \quad (\text{A5})$$

In (A5),  $n_p$  is the proton density,  $n_B$  the baryon density, and  $Y_p$  is the number of protons per baryon ( $Y_p = Y_{e^-} - Y_{e^+}$  = electrons per baryon minus positrons per baryon). If we define  $\bar{Y}$  to be the number of neutrinos per baryon minus antineutrinos per baryon, we obtain an equation analogous to (A5) for neutrinos:

$$\bar{Y} n_B = n_{\nu_e} - n_{\bar{\nu}_e}. \quad (\text{A6})$$

We note that the total lepton number per baryon is given by the sum of  $Y_p$  and  $\bar{Y}$ :

$$Y_p + \bar{Y} = (Y_{e^-} - Y_{e^+}) + (Y_{\nu_e} - Y_{\bar{\nu}_e}) = Y_L. \quad (\text{A7})$$

The energy density in the electron-positron gas is the sum of the energy density in electrons and the energy density in positrons. If we use (A1) for the energy densities and (A4) to relate the chemical potentials, we obtain

$$\varepsilon_e = \varepsilon_{e^-} + \varepsilon_{e^+} = \frac{T}{\pi^2} \left( \frac{T}{\hbar c} \right)^3 [F_2(\eta_e) + F_2(-\eta_e)], \quad (\text{A8})$$

where

$$\eta_e = \mu_{e^-}/T = -\mu_{e^+}/T. \quad (\text{A9})$$

Analogous equations hold for neutrinos.

Equation (A5) for the proton density may be combined with equations (A1) and (A4) to relate the electron chemical potential and the temperature:

$$Y_p n_B = \frac{1}{\pi^2} \left( \frac{T}{\hbar c} \right)^3 [F_2(\eta_e) - F_2(-\eta_e)]. \quad (\text{A10})$$

The analogous equation for neutrinos is

$$\bar{Y} n_B = \frac{1}{2\pi^2} \left( \frac{T}{\hbar c} \right)^3 [F_2(\eta_{\nu_e}) - F_2(-\eta_{\bar{\nu}_e})]. \quad (\text{A11})$$

Exact expressions have been derived by Bludman and Van Riper (1978) for the sum of Fermi integrals  $F_3(x) + F_3(-x)$  and the difference  $F_2(x) - F_2(-x)$ . Defining functions  $A(x)$  and  $B(x)$ , we find

$$A(x) = 3[F_2(x) - F_2(-x)] = x^3 + \pi^2 x, \quad B(x) = \frac{1}{\pi^2} [F_3(x) + F_3(-x)] = \frac{7\pi^2}{60} + \frac{1}{2}x^2 + \frac{1}{4\pi^2}x^4. \quad (\text{A12})$$

In terms of the functions  $A(x)$  and  $B(x)$  equations (A8) and (A10) may be written

$$Y_p n_B = n_{e^-} - n_{e^+} = \frac{1}{3\pi^2} \left( \frac{T}{\hbar c} \right)^3 A(\eta_e), \quad \varepsilon_e = \varepsilon_{e^-} + \varepsilon_{e^+} = \frac{T^4}{(\hbar c)^3} B(\eta_e). \quad (\text{A13})$$

The entropy density  $S_e$  of the electron-positron component may be calculated from the thermodynamic identity

$$\varepsilon_e = TS_e - P_e + (\mu_{e^-} n_{e^-} + \mu_{e^+} n_{e^+}). \quad (\text{A14})$$

Equation (A4) relating the chemical potentials of electrons and positrons, and the fact that the pressure of an ideal

relativistic gas is one-third the energy density, give

$$S_e = \frac{4}{3} \frac{\epsilon_e}{T} - \eta_e(n_{e+} - n_{e-}) . \quad (\text{A15})$$

This gives, using (A12) and (A13),

$$S_e = \frac{1}{3} \left( \frac{T}{\hbar c} \right)^3 \left[ \frac{7\pi^2}{15} + \eta_e^2 \right] . \quad (\text{A16})$$

The analogous equation for neutrinos is

$$S_\nu = \frac{1}{6} \left( \frac{T}{\hbar c} \right)^3 \left[ \frac{7\pi^2}{15} + \eta_\nu^2 \right] . \quad (\text{A17})$$

The entropy per baryon in electrons and neutrinos may be found by dividing the equations (A16) or (A17) for the entropy densities by the equations in (A13) giving the baryon density  $n_B$  in terms of  $T$ ,  $Y_p$ , or  $\bar{Y}$ , and  $\eta_e$  or  $\eta_\nu$ . For instance, we may divide (A17) for the entropy density in neutrinos by (A13):

$$\left( \frac{S_\nu}{n_B} \right) = \frac{Y_p}{2} \frac{[7\pi^2/15 + \pi^2\eta_\nu^2]}{\eta_e^3 + \pi^2\eta_e} . \quad (\text{A18})$$

The condition expressing the beta equilibrium of the neutron, proton, electron, and neutrino gas is the equality of the chemical potentials of reactants and products.

$$\mu_e - \mu_\nu = \mu_n - \mu_p \equiv \hat{\mu} . \quad (\text{A19})$$

If the neutron-proton gas is a nonrelativistic gas and we neglect the neutron-proton mass difference,  $\hat{\mu}$  may be written

$$\hat{\mu} = \mu_n - \mu_p = T \ln \left( \frac{1 - Y_p}{Y_p} \right) . \quad (\text{A20})$$

Dividing out the temperature, we obtain

$$\eta_e - \eta_\nu = \hat{\eta} = \ln \left( \frac{1 - Y_p}{Y_p} \right) . \quad (\text{A21})$$

The beta equilibrium of the matter may be cast into the form of a single cubic equation for  $\eta_e$  in terms of  $\hat{\eta}$ ,  $Y_p$ , and  $\bar{Y}$ . To obtain this cubic equation, write (A13) for the densities  $Y_p n_B$  and  $\bar{Y} n_B$ :

$$Y_p n_B = \frac{1}{3\pi^2} \left( \frac{T}{\hbar c} \right)^3 A(\eta_e) , \quad \bar{Y} n_B = \frac{1}{6\pi^2} \left( \frac{T}{\hbar c} \right)^3 A(\eta_\nu) . \quad (\text{A22})$$

The ratio  $Y_p / \bar{Y}$  is given by

$$A(\eta_e) - \frac{Y_p}{2\bar{Y}} A(\eta_\nu) = 0 . \quad (\text{A23})$$

Eliminate  $\eta_\nu$  from (A23) using the beta equilibrium equation (A21). The definition of the  $A$  functions, (A14), gives the desired cubic equation

$$\eta_e^3 - (3\beta\hat{\eta})\eta_e^2 + [\pi^2 + 3\beta\hat{\eta}^2]\eta_e - \beta A(\hat{\eta}) = 0 . \quad (\text{A24})$$

The parameter  $\beta$  is given by

$$\beta = Y_p / (Y_p - 2\bar{Y}) . \quad (\text{A25})$$

For electron degeneracy parameter  $\eta_e \leq 1$  the simple approximation

$$\eta_e \approx \beta\hat{\eta} , \quad (\text{A26})$$

is very useful. For  $\eta_e < 1$ , (A26) is good to better than 1%, but it breaks down rapidly for  $\eta_e > 1$ .

A useful special case of the equation of state is the one for which  $Y_p$  and  $\bar{Y}$  are given. For this case, which corresponds to an adiabat for the leptonic components of the gas, the parameters  $\eta_e$ ,  $\eta_\nu$  are fixed by (A24) and (A21). Thus the chemical potential of electrons and neutrinos scale with the temperature; e.g.,

$$\mu_e = \eta_e(Y_p, \bar{Y})T \quad (\text{adiabat}) . \quad (\text{A27})$$

TABLE 2  
EQUATION OF STATE

$Y_p$	$\bar{Y}$	$\beta$	$\hat{\eta}$	$\eta_e$	$\eta_v$	$(S/n_b)_L$	$k(Y_p, \bar{Y})$
0.39	-0.09	0.684	0.447	0.305	-0.142	8.87	5.72
0.36	-0.06	0.750	0.575	0.430	-0.145	5.84	8.81
0.33	-0.03	0.846	0.708	0.596	-0.112	3.89	13.6
0.30	0.00	1.00	0.847	0.847	0.000	2.52	21.9
0.27	+0.03	1.29	0.995	1.34	+0.348	1.49	42.6
0.24	+0.06	2.00	1.15	4.10	+2.95	0.608	335
0.23	+0.07	2.56	1.21	6.96	+5.75	0.402	1290
0.22	+0.08	3.67	1.27	12.0	+10.7	0.245	6160
0.21	+0.09	7.00	1.32	26.2	+24.9	0.114	63700
0.42	-0.09	0.700	0.323	0.226	-0.0971	12.9	3.91
0.39	-0.06	0.765	0.447	0.341	-0.106	7.94	6.41
0.36	-0.03	0.857	0.575	0.492	-0.0839	5.11	10.1
0.33	0.00	1.00	0.708	0.708	0.000	3.29	16.3
0.30	+0.03	1.25	0.847	1.09	+0.243	2.00	29.5
0.27	+0.06	1.80	0.995	2.41	+1.41	0.968	102
0.26	+0.07	2.17	1.05	4.15	+3.10	0.661	317
0.25	+0.08	2.78	1.10	7.00	+5.90	0.439	1210
0.24	+0.09	4.00	1.15	12.0	+10.9	0.268	5710
0.45	-0.09	0.714	0.201	0.143	-0.0574	21.7	2.31
0.42	-0.06	0.778	0.323	0.251	-0.0721	11.6	4.35
0.39	-0.03	0.867	0.447	0.387	-0.0604	7.01	7.29
0.36	0.00	1.00	0.575	0.575	0.000	4.38	12.0
0.33	+0.03	1.22	0.708	0.880	+0.172	2.68	20.8
0.30	+0.06	1.67	0.847	1.62	+0.775	1.44	49.6
0.29	+0.07	1.93	0.895	2.36	+1.46	1.07	92.1
0.28	+0.08	2.33	0.944	4.09	+3.14	0.726	285
0.27	+0.09	3.00	0.995	6.91	+5.92	0.483	1080
0.26	+0.10	4.33	1.05	11.9	+10.9	0.295	5120

The temperature  $T$  and baryon density  $n_b$  are related by (A13):

$$n_b = \frac{1}{3\pi^2 Y_p} A(\eta_e) \left( \frac{T}{hc} \right)^3. \quad (\text{A28})$$

In units convenient for the supernova problem we have

$$\rho_{10} = k(Y_p, \bar{Y}) \left( \frac{T}{10 \text{ MeV}} \right)^3 \quad (\text{A29})$$

with

$$k(Y_p, \bar{Y}) = 0.73 A(\eta_e) / Y_p. \quad (\text{A30})$$

The function  $k(Y_p, \bar{Y})$ , the ratios  $\eta_e$ ,  $\eta_v$ ,  $\hat{\eta}$ , and the total entropy per baryon in the leptons ( $e^+ e^- v_e \bar{v}_e$ ) are tabulated as functions of  $Y_p$  and  $\bar{Y}$ , in Table 2.

The equation of state for  $Y_p$  and  $\bar{Y}$  given is useful because the thermodynamic functions of the relativistic pair gas ( $e^+ e^- v_e \bar{v}_e$ ) are strong functions of  $Y_p$  and  $\bar{Y}$ , where those of the nonrelativistic nucleon gas are very weak functions of  $Y_p$ , and independent of  $\bar{Y}$ . We expect the total lepton number per baryon  $Y_L$  to be nearly constant, so calculating the equation of state for a given temperature, density, and lepton fraction means iterating the weak  $Y_p$  dependence in the nonrelativistic components with the strong dependence in the relativistic components.

The nucleon gas thermodynamic functions are given below:

$$P = n_b T = (\text{pressure}), \quad \epsilon = \frac{3}{2} n_b T = (\text{energy density}),$$

$$S = \frac{5}{2} + \ln \left[ \frac{mT}{2\pi\hbar^2} \right]^{3/2} \frac{1}{n_b} + Y_p \ln \left( \frac{1 - Y_p}{Y_p} \right) + \ln \left( \frac{1}{1 - Y_p} \right) = (\text{entropy per baryon}). \quad (\text{A31})$$

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**SN 1987A: An Empirical and Analytic Approach**  
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The concept of “gain radius” is introduced; outside the gain radius, neutrinos transfer more energy to matter than is lost by emission of neutrinos. It is concluded that about 1–2% of the total neutrino energy emitted by the core of the star can be transmitted to the matter. (Later calculations give higher efficiency for this energy transmission.)

## SN 1987A: AN EMPIRICAL AND ANALYTIC APPROACH

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### ABSTRACT

Starting from Wilson's idea that the supernova gets its energy from neutrinos heating the mantle of the star, I use the neutrino observations to find the available neutrino flux. This agrees well with recent computations by Wilson and Mayle, using "neutron fingers." In the mantle of the star, one can define a "gain radius;" outside this radius, the energy gain from neutrino absorption is greater than the energy loss by electron capture. The temperature and density are calculated from simple arguments for  $r > 100$  km: In the region where free nucleons dominate, the entropy is assumed to be constant; in the region where nucleons and  $\alpha$ -particles are mixed, the fraction of nucleons is determined from the internal energy. One can then calculate the fraction of neutrino energy which can be transferred to the region outside the gain radius; this turns out to be 1%–2%. With the observed neutrino flux, this gives a supernova energy of 0.8 foe (1 foe =  $10^{51}$  ergs); nucleosynthesis adds about 0.4 foe, for a total of 1.2 foe, compared with the observed energy of  $1.4 \pm 0.4$  foe.

In this paper, I shall try to go as directly as possible to the calculation of the supernova energy. Other problems are discussed in §§ 11–14. In particular, it is shown that, and why, the shock wave starts only after some delay.

*Subject headings:* stars: interiors — supernovae: individual (SN 1987A)

### 1. THE NEUTRINO MECHANISM

It seems pretty clear that supernovae of Type II, except perhaps the very light ones, work by means of Wilson's mechanism (Wilson 1982): neutrinos emitted by the core are absorbed in the mantle of the star, maybe at  $r = 100$ –300 km. They give their energy to the matter there, which then is expelled from the star.

It is important to have good information on the energy flux (luminosity) of the neutrinos. I propose that the most reliable information comes from the actual observations of neutrinos at Kamiokande (Hirata et al. 1987) and IMB (Bionta et al. 1987). This information is independent of models and of possible troubles in computation.

Only from SN 1987A do we have extensive observational information. But I am using this particular case to develop a theory for Type II supernovae in general. It may be objected that SN 1987A was not typical in being subluminous. This objection is not valid because light emission and the shock wave mechanism depend on different parts of the star.

Light emission depends on the hydrogen envelope of the progenitor. SN 1987A's progenitor was a blue, rather than a red, supergiant. It was of small size, therefore the radiating surface was small, and hence the light emission for the first two months was low. After about 2 months, the light emission became perfectly normal for a Type II supernova (SN). This complex of phenomena is explained in detail in the review article by Arnett et al. (1989).

The shock, on the other hand, is generated deep inside the star, in the core. The core is conveniently characterized by the mass of He (and heavier elements), which was somewhat under  $6 M_{\odot}$  for SN 1987A. This mass is related to the original mass of the star when on the main-sequence, which is believed to be about  $18 M_{\odot}$ . (Some of this mass,  $1$ – $2 M_{\odot}$ , was lost before the SN event; this is not relevant for the mass of the He core.)

Thus the different light curve is immaterial; for the shock formation, SN 1987A was a perfectly normal Type II SN.

Experience in past computations has shown that it is difficult to obtain the full observed energy from computations. Therefore, it appears that we should make use of as much neutrino flux as possible.

In this paper, I shall try to go as directly as possible to the calculation of the supernova energy. Issues like a theoretical model to explain the observed neutrino luminosity are postponed to the end of the paper (§ 11), as are the properties of the shock (§§ 12 and 13).

### 2. THE NEUTRINO OBSERVATIONS

The Kamiokande II collaboration (Hirata et al. 1987, 1988) observed 12 neutrinos from SN 1987A; the IMB collaboration (Bionta et al. 1987) detected 8. Both laboratories found a very high rate of events in the first 2 s, followed by a lower rate in the following 10. If we simply add the number of counts in the two laboratories, there are 14 in the first 2 s, or  $7 \text{ s}^{-1}$ , and 6 counts in the next 10 s, or  $0.6 \text{ s}^{-1}$ . Figure 1 shows the distribution of the counts in time.

Very early (Mayle & Wilson 1988) this was interpreted by attributing the high initial luminosity to accretion, and the lower, 10 s luminosity to the gradual cooling of the proto-neutron star. This interpretation has been generally accepted. We shall see (§ 7) that only the high-luminosity period is important for giving energy to the outgoing shock.

The two laboratories observe chiefly the capture of anti-neutrinos by protons,

$$p + \bar{\nu}_e \rightarrow n + e^+ . \quad (2.1)$$

Although about one event in each laboratory may have been due to the scattering of a neutrino ( $\nu$  or  $\bar{\nu}$ ) by an electron, we attribute all counts to reaction (2.1).

Hirata et al. (1988) give a curve of detection efficiency versus energy of the positrons emitted in reaction (2.1); when this is applied to their observations, one finds that 11 antineutrinos should have been detected in the first 2 s if the detector had

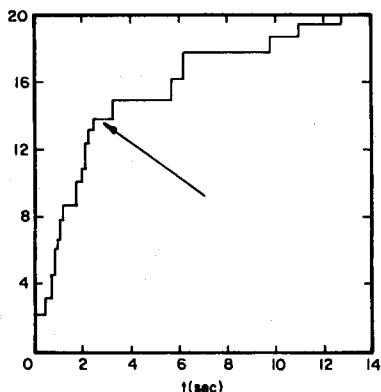


FIG. 1.—The (cumulative) number of neutrinos observed from SN 1987A, as compiled by Mayle & Wilson (1988). The arrow marks the transition from the initial period of very high luminosity (2 s) to the later period of lower luminosity.

100% efficiency. The average energy of the antineutrinos was

$$\epsilon = 15 \text{ MeV} = 2.4 \times 10^{-5} \text{ ergs} . \quad (2.2)$$

Using the cross section for reaction (2.1),

$$\sigma = 9.0 \times 10^{-44} \epsilon^2 \text{ cm}^2 \quad (2.3)$$

(where  $\epsilon$  is in MeV) and the fiducial volume of the detector,

$$2140 \text{ metric tons water} = 238 \text{ tons hydrogen} , \quad (2.4)$$

I find the fluence of the antineutrinos in the first 2 s to be

$$\Phi = 3.8 \times 10^9 \text{ cm}^{-2} \quad (2.5)$$

or the average flux

$$F = 1.9 \times 10^9 \text{ cm}^{-2} \text{ s}^{-1} . \quad (2.6)$$

The distance to the Large Magellanic Cloud is estimated to be  $D = 50$  kpc, hence the antineutrino luminosity (averaged over the first 2 s) is

$$L = 4\pi D^2 F \epsilon = 1.4 \times 10^{52} \text{ ergs s}^{-1} . \quad (2.7)$$

This is the luminosity in  $\bar{\nu}_e$ . Computations by Wilson & Mayle (1992) and by others have shown that the luminosities in  $\nu_e$  and  $\bar{\nu}_e$  are about the same, so the total luminosity in electron neutrinos,  $\nu_e + \bar{\nu}_e$ , is

$$L_{52} = 2.8 . \quad (2.8)$$

where  $L_{52}$  means the luminosity in units of  $10^{52}$  ergs  $s^{-1}$ . This gives a reasonable result for the total gravitational energy set free. In making this statement, I have assumed that the three flavors of neutrinos,  $\nu_e$ ,  $\nu_\mu$ , and  $\nu_\tau$ , share the released energy equally.

In the mantle of the SN, neutrinos can be captured by neutrons, antineutrinos by protons, so in § 4 we shall multiply the luminosity (2.8) by half the number of nucleons per cubic centimeter and by the cross section (2.3).

### 3. CONVECTION AND ACCRETION

As we mentioned, the initial, high neutrino luminosity is believed to be due to accretion. Some of the neutrinos are absorbed by the mantle of the star and thus supply energy to it.

This energy can be used most efficiently if it is convected to the outgoing shock. As discussed in § 1, to explain the observed energy of the supernova we should make use of as many neutrinos as possible.

This means we should have *simultaneously accretion and convection*. This is possible by making use of the massive convection model pioneered by Herant, Benz, & Colgate (1992). They showed, by a two-dimensional computation, that convection of the mantle will occur, and will be on a large scale.

In this picture, matter which has gone through the shock will flow inward and will there be heated by neutrinos. Some of this matter, due to the heating, will turn around, be further heated, and flow back out to the shock; in this way, neutrino heat is convected to the shock. But other parts of the ingoing stream will continue inward and accrete to the proto-neutron star; so we have simultaneously accretion and convection. The convection may look something like Figure 2, and may extend over a whole hemisphere (although that is not necessary for the success of the scheme).

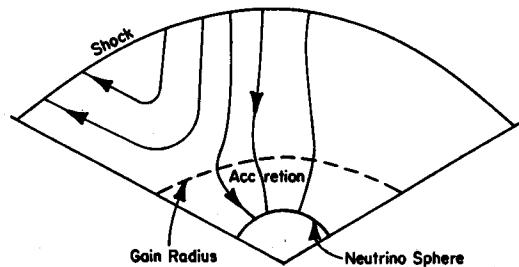
This picture may also make it understandable that accretion stops at some time. Indeed, in the computations of Herant et al., at some late time (which we would choose to be 2 s), the flow behind the shock becomes outward over the entire solid angle, there is no longer any part of the shock where the flow is inward. Just what causes this cessation of inward flow is not yet clear.

It would be interesting to know what fraction of the inward stream will accrete. The numerical simulation of Herant et al. (1992) is as yet unable to tell. We can get an idea by comparing two disparate calculations. One of these refers to the rate at which material is falling in from the outside and crosses the shock; the other is the computation of the growth of the proto-neutron star by Mayle & Wilson (1988).

Outside the shock, material is falling in with a velocity which is a fairly constant fraction of free-fall velocity, thus

$$u = \alpha(2GM/r)^{1/2} , \quad (3.1)$$

where  $M$  is the included mass and  $G$  the gravitational constant. In computations, such as those by Wilson & Mayle (1992)  $\alpha$  is usually about  $2^{-1/2}$  but its actual value will not be important in the following. Cooperstein et al. (1984) have shown that in these circumstances the material outside the shock gets thinner



Schematic of Flow Behind Shock

FIG. 2.—Schematic of the convection of material in the midlayers of a supernova. Material comes in from the outside and through the shock. In this picture, the material entering along the center line accretes to the star core at the neutrino sphere. Material entering near the sides of the sector shown is heated near the gain radius and turns around to go back toward the shock. Because the latter is supersonic, however, the material cannot go beyond the shock.

with time. If the original, presupernova material has a density distribution

$$\rho_0(r_0) = Hr_0^{-3}, \quad (3.2)$$

which is a reasonable approximation with  $H$  nearly constant, then the density outside the shock at time  $t$  (after the start of collapse) is

$$\rho(r) = \frac{2}{3} \frac{H}{\alpha(2GM)^{1/2}} t^{-1} r^{-3/2}. \quad (3.3)$$

The rate at which mass crosses the shock (rate of assembly) is then

$$\kappa = \frac{8\pi}{3} Ht^{-1}. \quad (3.4)$$

This is independent of  $\alpha$ , i.e., of the infall velocity.

The value of  $H$  has been computed by Woosley as a result of the presupernova evolution, making various assumptions concerning the cross section of the reaction  $^{12}\text{C}(\alpha, \gamma)^{16}\text{O}$  (Woosley & Weaver 1988). The result of one such calculation is shown in Bethe (1990, Fig. 22). For an enclosed mass of  $1.8 M_\odot$ ,

$$H = 6 \times 10^{31} \text{ g}. \quad (3.5)$$

Assuming that our accretion starts at  $t = 0.5$  (time after beginning of collapse) and lasts for 2 s, the infalling mass is

$$\begin{aligned} \Delta M &= (8\pi/3)H \ln(2.5/0.5) \\ &= 8 \times 10^{32} \text{ g} = 0.4 M_\odot. \end{aligned} \quad (3.6)$$

We call this the *assembled* mass; only part of it will be accreted.

An alternative way to calculate  $\Delta M$  is also based on Cooperstein, Bethe, & Brown (1984). The time  $t$  is related to the initial position  $r_0$  and the present position  $r$  of a given element of matter by

$$(2GM\alpha)^{1/2}t = \frac{1}{2}\pi r_0^{3/2} - \frac{2}{3}\pi r^{3/2}. \quad (3.7)$$

In this formula it has been assumed that  $r \ll r_0$ . With this assumption, we can calculate  $r_0$ . We take  $\alpha = 2^{-1/2}$ ,  $M = 1.8 M_\odot$ , and  $t = 2.5$ , and find

$$r_0 = 8500 \text{ km}. \quad (3.8)$$

Again using Woosley's computation,  $r_0 = 8500$  corresponds to an internal mass

$$M = 1.88 M_\odot. \quad (3.9)$$

In this calculation, the pre-SN mass of Fe is

$$M_{\text{Fe}} = 1.41 M_\odot. \quad (3.10)$$

It is reasonable to assume that this is the mass of the core at the time of bounce; then the mass assembled thereafter is

$$\Delta M = 0.47 M_\odot. \quad (3.11)$$

Wilson & Mayle (1992) find for the final mass of the proto-neutron star

$$M_{\text{WM}} = 1.66 M_\odot. \quad (3.12)$$

Taking their starting mass to be also given by equation (3.10),

$$\Delta M_{\text{WM}} = 0.25 M_\odot. \quad (3.13)$$

This would mean that about half the infalling mass accretes, while half stays in the convection region. But since these

numbers arise from totally different models, the result is rather unreliable.

#### 4. THE GAIN RADIUS

Two processes dominate in the material outside the neutrino sphere: the absorption of neutrinos and the capture of electrons and positrons. The first, essentially reaction (2.1), increases the energy of the material; the second decreases it. If they are calculated separately, the net energy absorbed is the difference between two large numbers.

This can be avoided by introducing the concept of the *gain radius*. The absorption of neutrinos is very nearly proportional to  $r^{-2}$ . The capture of electrons is nearly proportional to  $T^6$  (see eq. [4.2]), and this decreases much faster with  $r$  than  $r^{-2}$ . There will be a certain radius  $R_g$  where the two rates are equal. For  $r > R_g$ , the neutrino absorption dominates, therefore we have a net gain in energy. For  $r < R_g$ , the reverse is the case. We therefore call  $R_g$  the gain radius.

The rate of electron and positron capture per unit mass of material has been given by Herant et al. (1992) and is

$$\Lambda = 2.0 \times 10^{18} T^6 \Phi(\eta) \text{ ergs g}^{-1} \text{ s}^{-1}, \quad (4.1)$$

$$\Phi = 1 + (\eta^6 + 5\pi^2\eta^4 + 7\pi^4\eta^2)/1440, \quad (4.2)$$

where  $T$  is the temperature in MeV and

$$\eta = \mu/T, \quad (4.3)$$

with  $\mu$  the electron chemical potential.

The rate of neutrino absorption at distance  $r$  from the center of the star is

$$\Psi = \frac{\Lambda L}{4\pi r^2} \text{ ergs g}^{-1} \text{ s}^{-1}, \quad (4.4)$$

where  $L$  is the total luminosity of  $v_e + \bar{v}_e$  in ergs per second, and

$$A = \frac{1}{2} N_A \sigma_0 \epsilon^2 = 2.7 \times 10^{-20} \epsilon^2 \text{ cm}^2 \text{ g}^{-1}. \quad (4.5)$$

Here  $N_A$  is Avogadro's number,  $\sigma_0 \epsilon^2$  the absorption cross section per nucleon ( $\sigma_0 = 9 \times 10^{-44} \text{ cm}^2$ ), and  $\langle \epsilon^2 \rangle$  the average of the squared energy of the neutrinos. Neutrinos are absorbed by neutrons, antineutrinos by protons, and their numbers are assumed roughly equal, hence we use  $\frac{1}{2} N_A$  in equation (4.5).

The gain radius is determined by  $\Lambda = \Psi$ , hence

$$T^6 \Phi(\eta) r_g^2 = 0.11 \langle \epsilon^2 \rangle L_{52}, \quad (4.6)$$

where  $L_{52}$  is the neutrino luminosity in units of  $10^{52}$  ergs  $\text{s}^{-1}$ . The average  $\epsilon^2$  from the observations at Kamiokande is about  $250 \text{ MeV}^2$ , and a similar number follows from the numerical computations of Wilson & Mayle (1992), so

$$0.11 \epsilon^2 = 27. \quad (4.7)$$

Inside the gain radius, energy loss by electron capture would dominate if the left-hand side in equation (4.6) stayed constant. However, since there is no source of energy other than neutrinos,<sup>1</sup> the temperature will settle down so that the equilibrium equation (4.6) is fulfilled everywhere. Near the neutrino sphere, of course, the neutrino density is no longer proportional to  $r^{-2}$  but is somewhat larger because the neutrinos do not move radially outward, but we must still have  $\Lambda = \Psi$ , and

<sup>1</sup> This is different as long as accretion continues.

the temperature adjusts to a somewhat higher value than that in equation (4.6).

Obviously, to determine the gain radius, we need to know the temperature as a function of the radius. We shall obtain this in the next two sections, in § 5 for the region consisting mostly of nucleons and in § 6 for the region in which nucleons and  $\alpha$ -particles are mixed.

### 5. TEMPERATURE DISTRIBUTION

Outside the gain radius, we assume vigorous convection to take place, and, consequently, the entropy to be nearly independent of  $r$ , as it is in stellar evolution. (In fact, in the convective down stream the entropy should increase inward, due to neutrino heating, and in the up stream it should increase outward; on the average, there should be a rather small net decrease outward, to keep the convection going.)

In the inner part of this region, from about 100 to 200 km (as we shall show), the nuclear component is mostly in free nucleons. Their entropy is large but does not depend much on temperature and density; it is about 12 units per nucleon. The rest of the entropy, which is in radiation and electron pairs, is then also independent of  $r$ ; we call it the radiative entropy,  $S_r$ .

The star, behind (inside) the shock, is essentially in hydrostatic equilibrium,

$$-\frac{1}{\rho} \frac{dP}{dr} = \frac{GM}{r^2}. \quad (5.1)$$

This is because net accelerations must be much smaller than the gravitational acceleration, otherwise unreasonable velocities would soon be reached. The enclosed mass  $M$  is essentially independent of  $r$ ; we take it to be  $1.65 M_\odot$  on the basis of the calculations of Wilson & Mayle (1992). Then

$$GM = 2.2 \times 10^{26}. \quad (5.2)$$

We assume the boundary between nucleon and  $\alpha$ -particle regions to be at

$$T_a = 1 \text{ MeV}. \quad (5.3)$$

We estimate this boundary to be at a radius  $R_a$  of 200–300 km (§ 6).

The entropy (and other quantities) in the electron-positron gas are given by simple expressions, due to Bludman & Van Riper (1978). These formulae hold if  $T > \frac{1}{2}m_e c^2$ , which is the case in our conditions. Useful formulae derived from Bludman & Van Riper (1978) are given by Bethe, Applegate, & Brown (1980), to which we shall refer in the following. The entropy per unit volume is given by their equation (A16); it is (in units of  $k_B$ )

$$S_e = \frac{1}{3} \left( \frac{T}{\hbar c} \right)^3 \left( \frac{7\pi^2}{15} + \eta^2 \right). \quad (5.4)$$

The entropy in radiation is given by the same formula, with 7 replaced by 4, and  $\eta$  by 0.

The pressure is one-third of the energy density, given by equations (A12) and (A13) of Bethe et al. (1980). Including the radiation pressure, it is

$$P_r = \frac{T^4}{4(\hbar c)^3} \left( \frac{11\pi^2}{15} + 2\eta^2 + \pi^{-2}\eta^4 \right), \quad (5.5)$$

or in cgs units,

$$P_r = (1.26 + 0.35\eta^2 + 0.017\eta^4) 10^{26} T_{\text{MeV}}^4 \text{ dynes cm}^{-2}. \quad (5.6)$$

The theory also gives the number density of protons, being the difference between those of electrons and positrons. Assuming we know  $Y_p$ , the fraction of nucleons which are protons, we get the number density of nucleons,

$$n = \frac{1}{3Y_p} \left( \frac{T}{\hbar c} \right)^3 \eta \left( 1 + \frac{\eta^2}{\pi^2} \right). \quad (5.7)$$

Numerically, the density is

$$\rho_8 = 0.72 T_{\text{MeV}}^3 Y_p^{-1} \eta (1 + \eta^2/\pi^2). \quad (5.8)$$

The pressure in nucleons is

$$P_n = 0.96 \rho_8 T_{\text{MeV}} \times 10^{26} \text{ dynes cm}^{-2}, \quad (5.9)$$

and the total pressure is

$$P = (1.26 + 0.69\eta Y^{-1} + 0.35\eta^2 + 0.070\eta^3 Y^{-1} + 0.017\eta^4) \times 10^{26} T^4 \text{ dynes cm}^{-2}, \quad (5.10)$$

where  $Y = Y_p$ . The odd powers of  $\eta$  arise from the nucleons and the even ones from electrons and radiation.

Dividing equation (5.4) by equation (5.7), the entropy per nucleon in radiation plus electrons is

$$S_r = \pi^2 \frac{Y_p}{\eta} \frac{(11/15)\pi^2 + \eta^2}{\pi^2 + \eta^2}. \quad (5.11)$$

For  $\eta \ll \pi$ , this is

$$S_r = 7.2 Y / \eta \quad (Y = Y_p). \quad (5.12)$$

If we assume  $S_r = 5$ , then

$$\eta = 1.44 Y. \quad (5.13)$$

This is indeed  $\ll \pi$ , so that  $\eta^2$  and higher powers of  $\eta$  are unimportant. The values of  $\rho_8$  and  $P_{26}$  depend mainly on  $Y/\eta$ , not much on  $\eta$  and  $Y$  separately. We set

$$Y/\eta = b. \quad (5.14)$$

We insert equation (5.8), (5.10), and (5.2) in the hydrostatic equation (5.1), and get

$$\frac{dT}{dr} = -\frac{K}{r^2}, \quad (5.15)$$

$$K = 3.95 \left( \frac{1 + 0.101\eta^2}{1.26b + 0.69 + 0.35b\eta^2 + 0.070\eta^3 + 0.017b\eta^4} \right). \quad (5.16)$$

The solution of equation (5.15) is

$$T_{\text{MeV}} = K/r + \text{constant}. \quad (5.17)$$

The boundary condition which determines the constant is the inside radius of the  $\alpha$ -particle region, which will be determined in § 6. To derive the simple relation (5.17), we have only assumed hydrostatic equilibrium, and constant  $\eta$  and  $Y$ .

Using  $\eta/Y = 2.2$  from equation (6.10) and  $Y = 0.48$ , we find

$$K = 2.89. \quad (5.18)$$

The simple result in equation (5.17) is due to the fact that  $P/\rho$  is proportional to  $T$ , both for the nucleon contribution to pressure and for the contribution of radiation and electron pairs.

## 6. SPECIFIC ENERGY AND DENSITY

When the nucleons are combined in  $\alpha$ -particles, the entropy per nucleon is only about 3. In the mixed region in which there are both nucleons and  $\alpha$ -particles, the nuclear entropy changes greatly, from 12 to 3, and we therefore cannot expect the radiative entropy to stay constant. We therefore need a different argument to determine the physical conditions of the material as a function of radius.

The temperature is determined by the Saha equation. For simplicity, we assume it to be constant at  $T_e = 1.0$  MeV; instead of the temperature, we now have as a variable the fraction of free nucleons,  $X$ . The internal energy depends sensitively on  $X$ .

Infalling material starts out at a small (negative) total energy per unit mass (epm). As it moves inward, this epm does not change much. The gravitational potential energy,  $GM/r$ , is converted into internal and kinetic energy. Outside the shock, these share the energy roughly equally. Inside the shock, however, the kinetic energy is greatly diminished (typically, the infall velocity is reduced by a factor of 6, and the kinetic energy therefore by 36), so the  $GM/r$  all goes into internal, including thermal, energy. There will be some corrections due to work done by one mass element on another, but these should be small, and indeed are so in the computations by Wilson and collaborators.

I wish to determine the radius at which nearly all the material is in the form of free nucleons. I arbitrarily assume that the temperature there is 1.0 MeV. (In reality, according to the Saha equation, it is likely to be slightly higher.) Before collapse, the material at this point was mostly  $^{16}\text{O}$ , according to Woosley's computation of presupernova evolution. Therefore, the following amounts of energy are required (per nucleon)

To convert $^{16}\text{O}$ into $^4\text{He}$ :	0.90 MeV
To convert $^4\text{He}$ into $\text{H} + n$ :	7.07 MeV
To give the nucleons a temperature of 1 MeV:	1.50 MeV
To give the electron-positron gas a temperature of 1 MeV:	$\sim 1.1$ MeV

Then the total energy required is

$$\epsilon = 10.6 \text{ MeV nucleon}^{-1}. \quad (6.1)$$

Setting this equal to the gravitational potential energy of a nucleon,

$$V = GM/r, \quad (6.2)$$

and assuming  $M = 1.65 M_\odot$  (following the computations of Wilson & Mayle), we get

$$r = 207 \text{ km}. \quad (6.3)$$

This permits us to determine the constant in equation (5.17), which now reads

$$T = \frac{2.89}{r_7} - 0.39. \quad (6.4)$$

In  $\alpha$ -particles, the neutrino absorption is very small, as is also the electron capture. Thus the net neutrino absorption is proportional to the fraction  $X$  of free nucleons. The point where  $X = \frac{1}{2}$  is given by a similar calculation to that above,

but with the following energy requirements:

To convert one-half of $^4\text{He}$ into $\text{H} + n$ :	3.54 MeV
To give nucleons and $\alpha$ 's $T = 1$ MeV:	0.94 MeV
For the electron-positron gas, estimated:	$\sim 2.2$ MeV.

This gives

$$\epsilon = 7.6 \text{ MeV}, \quad r = 300 \text{ km}. \quad (6.5)$$

The density outside the shock is derivable from the rate of accretion (eq. [3.4]); Cooperstein et al. (1984) find

$$\rho_1 = \frac{2}{3} \frac{H t^{-1}}{\alpha (2GM)^{1/2} r^{3/2}}. \quad (6.6)$$

Using  $H = 6 \times 10^{31}$ ,  $\alpha = 2^{-1/2}$ , and  $r = 207$  km,

$$\rho_1 = 2.9 \times 10^7. \quad (6.7)$$

The density behind the shock is typically about 6 times larger than in front, giving

$$\rho_2 = 1.75 \times 10^8. \quad (6.8)$$

As long as we have accretion (as we have assumed), it is reasonable to assume this result to hold approximately. There are complications: we have both a down stream and an up stream of particles, and the shock is complicated in the presence of massive convection. Thus the result for the density is less reliable than that for the temperature.

The density (eq. [6.8]) is rather low, and is in the range where material and radiative pressure are comparable, so that § 5 applies. Using equation (5.8),

$$\eta/Y = 2.2. \quad (6.9)$$

Choosing  $Y = 0.48$ , we have

$$\eta = 1.05, \quad (6.10)$$

which is small compared with  $\pi$ . The energy derivable from neutrino absorption is roughly proportional to the matter density, hence it is essential that the absorption region lie *behind* the shock so that it benefits from the enhanced density  $\rho_2$ . The effective absorption region extends out to the place where one-half the matter is in free nucleons and one-half in  $\alpha$ -particles. Therefore, it is essential that the prompt shock should survive beyond that boundary, i.e., beyond 300 km. This conclusion was reached long ago by Wilson on the basis of his computations.

The radiative entropy per nucleon is

$$S_r = 5.2 T^3 / \rho_8. \quad (6.11)$$

In our case,  $T = 1$  MeV and  $\rho_8 = 1.75$ , so

$$S_r = 3. \quad (6.12)$$

Wilson and Mayle, in their computation of 1992 March 26 (private communication), find an  $\eta/Y$  which corresponds to  $S_r = 3$ ; this is in agreement with equation (6.12), even though their assumptions are somewhat different from ours.

## 7. DETERMINATION OF THE GAIN RADIUS

The gain radius and temperature are determined by the equilibrium equation (4.6). In accord with equation (6.10), we choose  $\eta = 1.05$ ; then from equation (4.2) we get

$$\Phi(\eta) = 1.53. \quad (7.1)$$

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It is then convenient to take the square root of equation (4.6), inserting equation (4.7)

$$T^3 r_\gamma = 4.2 L_{52}^{1/2}. \quad (7.2)$$

We use equation (6.4), and the observed  $L$  (eq. [2.8]), which yields

$$T_\theta = 1.72 \text{ MeV}. \quad (7.3)$$

Using equation (6.4) again, the gain radius is

$$R_g = 137 \text{ km}. \quad (7.4)$$

Obviously,  $T_\theta$  must be greater than 1 MeV; otherwise there is no region of energy gain at all. Furthermore, in equation (8.8) we show that the fraction of neutrino energy transmitted to matter is proportional to  $(1 - T_a^2/T_\theta^2)^2$ , so it is very small if  $T_\theta$  is close to  $T_a \approx 1$  MeV. To get appreciable energy, we may require, e.g., that

$$T_\theta^2 > 2; \quad (7.5)$$

then equation (7.2) requires that

$$F_{52} > 1.16. \quad (7.6)$$

Thus the delayed shock will not get started unless the neutrino flux is quite large. This may explain why several authors were unable to find shock revival.

Inside the gain radius, the temperature is given by equation (4.6). Since the right-hand side is constant, and as long as  $\Phi(\eta)$  is also constant, we have

$$T \sim r^{-1/3}, \quad (7.7)$$

a very slow temperature variation. Taking the radius of the neutrino sphere to be 20 km, and using inequality (7.5), the temperature increases by approximately 80% from the gain radius to the neutrino sphere, which gives about 3.3 MeV at the latter, appreciably short of the correct temperature (5 MeV).

The entropy is of course not constant in this region, but decreases toward the center. Inserting equation (4.6) in the hydrostatic equations (5.1), and using the expressions for density and pressure derived in § 5, it is possible to calculate the distribution of density, pressure, and of course  $\eta$  in the region between neutrino sphere and gain radius. But this will not have an appreciable influence on the energy given to the shock; this is determined by the region outside the gain radius.

The collision between neutrinos,

$$v + \bar{v} = e^+ + e^-, \quad (7.8)$$

has been suggested by Goodman, Dar, & Nussinov (1987) in order to supply extra energy to the shock, and is used by Wilson & Mayle (1989). Its contribution to energy goes as

$$w(v\bar{v}) \sim (R_w/r)^8, \quad (7.9)$$

where  $R_w$  is the radius of the neutrino sphere. We have shown that only energy deposited outside the gain radius contributes to the shock, and with our values for  $R_g$  and  $R_w$ ,

$$w(v\bar{v}) \sim 6^{-8} \sim 10^{-6}. \quad (7.10)$$

## 8. ENERGY SUPPLY

Neutrino energy deposited outside the gain radius can be brought to the shock by convection. The cross section for absorption of neutrinos is given by equation (4.5), and we have

chosen  $\epsilon^2 = 250$ , so that

$$A = 6.7 \times 10^{-18} \text{ cm}^2 \text{ g}^{-1}. \quad (8.1)$$

The fraction of the neutrino energy absorbed is then

$$\alpha = 6.7 \times 10^{-18} \int \rho dr, \quad (8.2)$$

where the integral extends from the gain radius  $R_g$  to the boundary of the  $\alpha$ -particle region,  $R_\alpha$ .

We insert the expression for the density, equation (5.8), setting  $1 + \eta^2/\pi^2 = 1.11$ , getting

$$100\alpha = 0.53(\eta/Y) \int T^3 dr_\gamma. \quad (8.3)$$

To facilitate analytic integration, I approximate equation (6.4) by

$$T = 2.23/r_\gamma, \quad K = 2.23. \quad (8.4)$$

This gives the correct answer at 170 km, in the middle of the relevant region. Then we get

$$100\alpha = \int_{T_a}^{T_\theta} 0.53(K\eta/Y)T dT = 0.27(K\eta/Y)(T_\theta^2 - T_a^2). \quad (8.5)$$

This gives the percentage of neutrino energy absorbed.

We must subtract from this the energy loss due to electron capture. We know that at the gain radius this is equal to the energy gain due to neutrino absorption, and its ratio to that gain is given by the left-hand side of equation (4.6); hence the integral in equation (8.5) is to be replaced by

$$\int_{T_a}^{T_\theta} \frac{T^6 r^2}{T_\theta^6 R_g^2} T dT = \int_1^{T_\theta} \frac{T^5}{T_\theta^4} dT = \frac{1}{6} (T_\theta^2 - T_a^{-4} T_a^6), \quad (8.6)$$

where we have again used equation (8.4). Subtracting this from equation (8.5), we get

$$100\alpha = 0.088(K\eta/Y)(2T_\theta^2 - T_a^2 + T_a^6 T_\theta^{-4}) \quad (8.7)$$

$$= 0.088(K\eta/Y)(1 - T_a^2/T_\theta^2)^2(2T_\theta^2 + T_a^2). \quad (8.8)$$

Inserting  $K$  from equation (8.4),  $\eta/Y$  from equation (6.10),  $T_a$  from equation (7.3), and  $T_a = 1$ , we get

$$100\alpha_1 = 1.30. \quad (8.9)$$

To this must be added the contribution from the region in which some of the nucleons are combined into  $\alpha$ -particles. In this region, the neutrino absorption is proportional to  $X$ , the fraction of nucleons. Instead of calculating this explicitly, we assume that the region with  $X > \frac{1}{2}$  contributes fully and the region  $X < \frac{1}{2}$  not at all. We found in equation (6.5) that  $X = \frac{1}{2}$  is located at  $R_2 = 300$  km, while full dissociation into nucleons occurs at  $R_1 = 207$  km (eq. [6.3]).

In the region  $X > \frac{1}{2}$ , we assume that  $T^3 r_\gamma$  is constant and equal to its value at  $T_a$ , which is

$$T_\theta^3 r_{\gamma_\alpha} = (T_\theta r_{\gamma_\alpha}) T_\theta^2 = (T_\theta r_{\gamma_\alpha})(T_\theta^2/T_\theta^2), \quad (8.10)$$

since  $T r_\gamma$  is constant between  $T_a$  and  $T_\theta$ . Now the ratio of electron capture to neutrino absorption is proportional to the square of  $T^3 r$  (see the beginning of § 7), and the ratio is unity when  $T^3 r = T_\theta^3 r_\theta$ . Therefore, the net energy deposited is related to the gross energy delivered by the neutrino by the

factor

$$F = 1 - (T_e/T_g)^4. \quad (8.11)$$

The gross energy is given by equation (8.2), where the integral now extends from  $R_1$  to  $R_2$  (see above). Let us assume that the density in this region is proportional to  $r^{-3/2}$ , as in equation (6.7); then

$$\begin{aligned} \int_{R_1}^{R_2} \rho dr &= \rho(R_1) \int (R_1/r)^{3/2} dr \\ &= \rho(R_1) R_1 \times 2[1 - (R_1/R_2)^{1/2}] \\ &= \rho(R_1) R_1 \times 0.34, \end{aligned} \quad (8.12)$$

using  $R_1 = 207$ ,  $R_2 = 300$ . Using equation (5.8) for the density, and equation (8.2),

$$100\alpha = 0.53(\eta/Y)T_e^3 R_{1,7} \times 0.34F. \quad (8.13)$$

Inserting values, and using equation (8.11),

$$100\alpha_2 = 0.73. \quad (8.14)$$

Adding to this equation (8.9), we get

$$100(\alpha_1 + \alpha_2) = 2.03. \quad (8.15)$$

Absorption of neutrinos by nucleons thus has an efficiency of about 2%. The region which is fully dissociated into nucleons contributes about twice as much as the partially dissociated region.

Equation (8.15) is the net percentage of neutrino energy transmitted to the convection region via absorption by nucleons. To this we may add the neutrino energy absorbed by electrons via elastic scattering. This process will be discussed in § 10; it contributes about 0.11% to the efficiency. The total is then 2.14%.

However, not all the energy deposited in the mantle of the star will go into the shock. As we know, in the convection there is a down stream and an up stream. Part of the material in the down stream (maybe one-half) will accrete, and the rest will go into the up stream and hence into the shock. If we guess the accreting part of the down stream to be one-half, it is reasonable to estimate that two-thirds of the energy will go into the shock. Hence our best guess for the net efficiency of neutrino energy absorption is

$$100\alpha_{\text{eff}} = 1.4. \quad (8.16)$$

## 9. SUPERNOVA ENERGY

In § 2 we calculated from the Kamiokande observations that the energy in  $v_e + \bar{v}_e$  is  $5.6 \times 10^{52}$  ergs in the first 2 s. At the end of § 8, we calculated that about 1.4% of that energy is given to the shock. Thus the shock energy is

$$E = 0.8 \text{ foe}, \quad (9.1)$$

clearly with wide limits of error.

This is of the same order of magnitude, but rather smaller than the observed energy (Bethe & Pizzichero 1990),

$$E_{\text{obs}} = 1.4 \pm 0.4 \text{ foe}. \quad (9.2)$$

Some increase of the theoretical energy will result from the fact that the neutrino luminosity is not constant but is higher in the first half-second than in the following 1.5 s. The energy is not linear in the integrated neutrino luminosity, hence nonuniformity leads to higher total energy. However, we disregard this effect.

Nucleosynthesis will help: Initially, the material outside the final proto-neutron star is mostly  $^{16}\text{O}$ . We know that  $0.075 M_\odot$  of this is converted into  $^{56}\text{Ni}$ , giving an energy of 0.11 foe. It is reasonable to assume that an additional  $0.3 M_\odot$  is transformed into  $^{28}\text{Si}$  and  $^{32}\text{S}$ , a process which releases an additional 0.28 foe. Adding these to the above energy from neutrino absorption gives a total energy

$$E = 1.2 \text{ foe}, \quad (9.3)$$

in good agreement with the observations.

However, it is clearly important to get as much energy as possible from neutrino absorption, and in particular to make use of the entire 2 s of high neutrino luminosity: on the other hand, neutrinos arriving after 2 s will not be effective because of their low luminosity. Further, it would be good to keep the density in the mantle high, which means to keep the entropy low; this may be facilitated by the massive convection of Herant et al.

In the remainder of this paper, I shall discuss some other effects.

## 10. COLLISIONS BETWEEN NEUTRINOS AND ELECTRONS

This process has been calculated by Tubbs & Schramm (1975). Their formulae can be substantially simplified if electron and positron energies are greater than  $m_e c^2$ , which is the case in our problem. Further simplification results if  $\mu_e \approx 0$ , which is also true, since our  $\eta$  is small; then the collision rate of any  $v_e$  or  $\bar{v}_e$  with the gas of electrons and positrons is

$$\kappa = 2.7 \times 10^{-12} \epsilon_e T^4 \text{ cm}^2 \text{ cm}^{-3}. \quad (10.1)$$

It is, of course, independent of the material density  $\rho$ . In the collision, if  $\epsilon_e \gg T$ , half the neutrino energy is transferred to the electron or positron. Setting  $\epsilon_e = 15$ , as before, the energy transfer rate is then

$$\kappa' = 2.0 \times 10^{-11} T^4 \text{ cm}^2 \text{ cm}^{-3}. \quad (10.2)$$

There is a corresponding energy loss due to neutrino pair production,

$$e^+ + e^- \rightarrow v + \bar{v}. \quad (10.3)$$

This energy loss has been discussed, on the basis of earlier work, by Bethe et al. (1980), and is

$$-\dot{\omega}_p = 1.0 \times 10^{25} T^9 \text{ ergs cm}^{-2} \text{ s}^{-1}. \quad (10.4)$$

Its ratio to the energy gain (eq. [10.2]) is similar to that of electron capture to neutrino capture by nucleons. So we may calculate the gain due to equation (10.2) from the gain radius on out, and then correct it, similar to the procedure in equation (8.5).

According to equation (10.2), the fraction of neutrino energy absorbed by electrons and positrons is

$$\alpha_2 = 2.0 \times 10^{-11} \int \frac{4\pi r^2 dr}{4\pi r^2} T^4. \quad (10.5)$$

Inserting equation (8.4) in equation (10.5) and using  $R_2/R_1 = 1.38$ ,

$$100\alpha_e = (0.020/3)K(T_e^3 + 0.14T_g^3) = 0.09. \quad (10.6)$$

To this we may add the contributions of  $\mu$ - and  $\tau$ -neutrinos. The energy flux in each of these is about the same as in  $e$ -neutrinos. The cross section is about one-sixth of that for  $v_e$ , but the average energy is about 50% larger. Together, these

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two species then add 50% to expression (10.6). On the other hand, for the process (10.3) we should subtract about 33%, giving for the net contribution from electron collisions

$$0.11\%. \quad (10.7)$$

## 11. NEUTRON FINGERS

Wilson and Mayle recognized early the importance of high neutrino flux for a successful shock. In their computations, the neutrinos from accretion were not sufficient. They needed, in addition, to enhance the flow of neutrinos from the core of the star.

They find a region in the star where  $Y_e$  is nearly constant. (In their computation of 1992 March 26 [private communication], this region extends from  $M_1 = 1.0$  to  $M_2 = 1.45 M_\odot$ .) Inside  $1.0 M_\odot$ ,  $Y_e$  is high, generally 0.2–0.3; outside  $1.5 M_\odot$  it is low because the neutrinos can easily escape from there, and thus electron capture is strong. This situation is unstable because a region of small  $Y_e$  has, at given pressure, a higher density than a region of large  $Y_e$ , hence it tends to fall to the center.

They propose that equilibrium is established by the formation of "neutron fingers" in the region of overall constant  $Y_e$ . In a horizontal plane (actually, a spherical shell), neutron-rich areas (relatively small  $Y_e$ ) form, alternating with neutron-poor areas. These areas are rather small in the horizontal plane, but vertically they extend all the way from the high- $Y_e$  to the low- $Y_e$  region. The neutron-poor areas obtain considerable pressure from their electrons, and hence need relatively low density to have the same total pressure as the low- $Y_e$  areas in the same horizontal plane. Hence the high- $Y_e$  areas are buoyant and tend to rise, transporting high- $Y_e$  material from inside to the neighborhood of the neutrino sphere. This material then has enhanced electron capture and gives rise to enhanced neutrino emission.

In a Report on the Progress of Supernova Research (Wilson & Mayle 1992) the authors treat this process by dimensional analysis which leads to a formula for the effective diffusion coefficient of neutrons (or  $Y_e$ ). They determine a numerical factor in this formula so as to get best agreement with observations. With this factor, the neutron fingers contribute about 10% to the overall neutrino luminosity. This is of the same order as the observed luminosity after the end of accretion.

## 12. START OF THE SHOCK

In many computations, the revived shock failed to get started. In this section we investigate the conditions for a start.

Obviously, the shock pressure must be high enough so that the shock velocity relative to the center of the star is positive or at least zero

$$U = U' - u > 0, \quad (12.1)$$

where  $u$  is the infall velocity of the material outside the shock (eq. [3.1]) and  $U'$  is the shock velocity relative to the infalling material. This is given by the Hugoniot relation,

$$U'^2 = 6P_S/5\rho_1 \quad (12.2)$$

where we have assumed, as in equation (6.9), that the density increases in the shock by a factor of 6. The density outside the shock,  $\rho_1$ , is given by equation (6.7). Inserting equations (3.1) and (6.7) in equation (12.2),

$$P_S > \frac{5}{6} \rho_1 u^2 = \frac{5}{9} \frac{H\alpha(2GM)^{1/2}}{R_S^{5/2} t}. \quad (12.3)$$

Using  $\alpha = 2^{-1/2}$ ,

$$P_S R_S^3 > \frac{5}{9} (GM)^{1/2} H t^{-1} R_S^{1/2}. \quad (12.4)$$

We can relate  $P_S R_S^3$  to the same quantity at the gain point which we can calculate from § 7. The relation is provided by the virial theorem, which holds in the absence of accelerations, i.e., in hydrostatics. Cooperstein et al. (1984) have put this in the form

$$4\pi(P_B R_B^3 - P_A R_A^3) = V + 3W, \quad (12.5)$$

$$V + 3W = \int_A^B \left[ \frac{3P}{\rho} - \frac{GM(r)}{r} \right] dM. \quad (12.6)$$

We choose A to be the gain point, and B the shock. The pressure at the gain point is

$$P_g = 1.25 \times 10^{26} T_g^4 (1 + 4/S_g) = 2.6 \times 10^{27} \text{ ergs cm}^{-3}, \quad (12.7)$$

where  $4/S_g$  is the ratio of material to radiation pressure, and we have used equation (7.3) for  $T_g$  and equation (6.13) for  $S_g$ . Using equation (7.4) for  $R_g$ ,

$$P_g R_g^3 = 6.6 \times 10^{48} \text{ ergs}. \quad (12.8)$$

Similarly, setting  $H = 10^{32} h$ , and inserting  $GM = 2.2 \times 10^{26}$ , equation (12.4) becomes

$$P_S R_S^3 > 2.6 \times 10^{48} h t^{-1} R_S^{1/2} \quad (12.9)$$

To calculate the virial (eq. [12.6]), we first calculate the mass between  $R_g$  and  $R_S$  using the density in equation (3.3). We multiply this by 6 to take into account the fact that the density increases by a factor of 6 behind the shock; thus

$$\frac{M_{AB}}{4\pi} = \int 6\rho_1 r^2 dr = \frac{4Ht^{-1}}{(GM)^{1/2}} \frac{2}{3} (R_S^{3/2} - R_g^{3/2}). \quad (12.10)$$

We set again  $H = 10^{32} h$  and find

$$M/4\pi = 0.56 \times 10^{30} h t^{-1} (R_S^{3/2} - R_g^{3/2}). \quad (12.11)$$

The coefficients in the virial (eq. [12.6]) are given in Table 1 in units of  $10^{18} \text{ ergs g}^{-1}$ , at several values of  $R$ ; cf. §§ 6 and 7.

In calculating  $P/\rho$ , we assumed the values from §§ 5 and 6, i.e., the initial values before the material is heated by neutrinos. At this time,  $3P/\rho$  is only about half of  $GM/r$ , so the virial is negative. Specifically, in calculating  $P/\rho$  for the smaller radii, we assumed that the material is pure nucleons; then the material pressure is

$$P_m/\rho = 0.96 \times 10^{18} T_{MeV}, \quad (12.12)$$

and the radiation pressure is given by  $P_r/P_m = S_r/4$ . At 300 km the material is half nucleons and half  $\alpha$ -particles; then the material pressure is five-eighths of expression (12.12), while the radiation pressure is unchanged.

TABLE 1  
VIRIAL COEFFICIENTS

$R$ (km)	$T$ (MeV)	$GM/r$	$3P/\rho$	$GM/r - 3P/\rho$
116.....	1.82	19.0	9.2	9.8
207.....	1.0	10.6	5.0	5.6
300.....	1.0	7.3	4.0	3.3

Using equation (12.11) and Table 1,

$$(V + 3W)/4\pi = 12.9 \times 10^{48} ht^{-1} \text{ if } R_s = 300 \text{ km} . \quad (12.13)$$

Note that this as well as the shock pressure (12.9) are proportional to  $ht^{-1}$ , and that the shock pressure is considerably less than the virial (12.13). Adding formula (12.9) with an equality sign to equation (12.13) and equating the sum to expression (12.8), we find that

$$ht^{-1} = 0.38 . \quad (12.14)$$

This, then, is the maximum value of  $ht^{-1}$  for which the shock can move outward from 300 km before neutrino heating.

Reasonable values for  $h$  are 0.4–0.6, so the shock could not get started before  $t = 1$  or 1.6 s. This may explain the failure of many computations, but it is very unsatisfactory because at  $t = 2.5$  s the strong neutrino luminosity stops.

Fortunately, neutrino heating will increase  $P/\rho$ . According to our earlier discussion, the neutrino energy is added exactly in the region between gain point and shock. Some of this added energy  $\Delta E$  goes into radiation, some into nuclear energy. For the radiation,  $\Delta E_r = 3\Delta P_r/\rho$ . For the nuclear energy in the region which is already fully dissociated into nucleons,  $\Delta E_n = (3/2)\Delta P_n/\rho$ , so  $3\Delta P_n/\rho > \Delta E_n$ . For the region which is mixed  $\alpha$ -particles and nucleons, most of the added energy goes into further dissociation of  $\alpha$ -particles, so  $3\Delta P_\alpha/\rho \ll \Delta E_n$ . Adding all parts together, probably

$$3\Delta P/\rho = \Delta E . \quad (12.15)$$

We shall assume this to be correct.

We have found that the total energy deposited by neutrinos is 0.8 foe in 2 s,

$$\Delta E = 4 \times 10^{50} \text{ ergs s}^{-1} . \quad (12.16)$$

The amount of mass between  $R_g$  and  $R_s$  is irrelevant here, and we get

$$3\Delta W/4\pi = 3 \times 10^{49}(t - t_0) , \quad (12.17)$$

where  $t_0$  is the time (after beginning of collapse) when neutrino heating begins. So, putting together formulae (12.9), (12.13), (12.8), and (12.17), the time of the start of the shock is given by

$$1.74ht^{-1} = 0.66 + 3(t - t_0) . \quad (12.18)$$

The solution is given in Table 2, assuming  $t_0 = 0.5$ .

There is always a delay between neutrino heating and the start of shock. The delay is shortest if the infalling material is already dilute before collapse. The start of shock is produced by a combination of dilution of the infalling material and increase of energy in the material between gain point and shock.

Before its "start," the shock recedes. We cannot derive, at present, the radius at which it finally turns around. Clearly, the start is a struggle between the energy behind the shock and the

TABLE 2  
TIME OF START OF SHOCK, AFTER START  
OF NEUTRINO HEATING

PARAMETER	$h$				
	0.3	0.4	0.6	0.8	1.0
$t - t_0$ .....	0.07	0.13	0.24	0.33	0.42
$P_s R_s^2$ .....	2.4	2.9	3.8	4.4	5.0

velocity of the infalling material, so the shock must start slowly. This is not apparent in the existing computations, probably because the shock in these is smeared out by artificial viscosity.

The addition of energy means that the temperature at any given  $r$  is higher than in § 6. This is easily accommodated in equation (6.4) by a positive integration constant,

$$T = K/r_7 + B, \quad B > 0 . \quad (12.19)$$

$B$  will increase with time. There will also be an effect on the gain temperature.

The last line in Table 2 gives  $P_s R_s^3$ ; it increases with  $h$ . This is to be expected, because the larger  $h$  is, the more pressure in the shock is required to push ahead. Quite generally, however,

$$P_s R_s^3 < P_\theta R_\theta^3 . \quad (12.20)$$

Thus the virial  $V + 3W$  is always negative in this range of  $h$ . Crudely speaking, the internal energy  $W$  does not fully make up for the negative potential energy. But it does so partially. The neutrino energy deposition serves to replenish the internal energy which was depleted by the dissociation of the initial  $^{16}\text{O}$  into nucleons.

### 13. THE SHOCK

Once the shock has progressed beyond, say, 1000 km, its pressure can be deduced from the net ram concept of Cooperstein et al. (1984). Rewriting their equation (3.5), we have

$$4\pi P_s R_s^3 - 4\pi P_\theta R_\theta^3 = E - \int_g^s (\epsilon - 3p/\rho)dM , \quad (13.1)$$

where  $E$  is the total energy between gain radius and shock, i.e., the energy which will ultimately be available to the shock.

In the integral,  $\epsilon$  is the internal energy per unit mass. Energy in radiation (including electron pairs) need not be counted because it is exactly canceled by the radiation part of  $3p/\rho$ . For the nuclear material, we take  $^{16}\text{O}$  at rest. Then, in the region where the material is nucleons,

$$\epsilon - \frac{3p}{\rho} = D_n + (\frac{3}{2})\frac{p}{\rho} - \frac{3p}{\rho} = D_n - (\frac{3}{2})0.96 \times 10^{18} T_{\text{MeV}} , \quad (13.2)$$

where  $D_n$  is the dissociation energy of  $^{16}\text{O}$  into nucleons,

$$D_n = 8.0 \text{ MeV} = 7.68 \times 10^{18} \text{ ergs g}^{-1} . \quad (13.3)$$

We may set  $T_{\text{MeV}} = 1.5$  in this region. In the  $\alpha$ -particle region,

$$\epsilon - 3p/\rho = D_\alpha - (\frac{3}{2})0.96 \times 10^{18} T_{\text{MeV}} , \quad (13.4)$$

$$D_\alpha = 0.90 \text{ MeV}, \quad T = 0.75 \text{ MeV} . \quad (13.5)$$

The mass in the nucleon region can be calculated from equation (12.11). We now set  $R_7 = 3$ ,  $t = 1.5$ , and  $h = 0.6$  (the latter because  $h$  increases with  $t$ ), and find

$$M_n = 1.0 \times 10^{31} \text{ g} , \quad (13.6)$$

only half a percent of a solar mass. The  $\alpha$ -particle region we estimate to extend from 300 to 600 km; its mass is then

$$M_\alpha = 2.5 \times 10^{31} \text{ g} . \quad (13.7)$$

Thus

$$\int (\epsilon - 3p/\rho) dM = 5.5 \times 10^{49} \text{ ergs}. \quad (13.8a)$$

In the nucleon region,

$$\int_a (\epsilon - 3p/\rho) dM = 1.5 \times 10^{49} \text{ ergs}. \quad (13.8b)$$

As the shock progresses, the masses in the nucleon and  $\alpha$ -region may diminish further. Using equations (12.8) and (13.8), equation (13.1) yields

$$4\pi P_s R_s^2 = E - 0.01 \text{ foe}. \quad (13.9)$$

A result similar to this has long been used in papers on nucleosynthesis. Using the approximate equality

$$w = 3P, \quad (13.10)$$

where  $w$  is the energy per unit volume, equation (13.9) says that this energy density behind the shock is very nearly equal to the total energy divided by the total volume covered by the shock.

Our derivation has the advantage over previous ones that it includes the corrections due to nuclear dissociation as well as those due to gravitation, which are quite large: at the gain radius, the gravitational energy per nucleon is nearly 20 MeV! The correction term is accidentally very near zero though of course very uncertain, but it is clearly only a small fraction of  $E$ .

The shock energy  $E$  increases, as the neutrinos feed energy in. If we assume constant shock velocity,  $E$  also increases linearly with  $R_s$ .

When the shock has its full energy, we set

$$E' \equiv E - 0.01 = 1.0 \text{ foe}. \quad (13.11)$$

In the bulk of the presupernova He, according to Woosley,

$$H = 2 \times 10^{32} \text{ g} \quad (13.12)$$

(see Bethe 1990, Fig. 22). Then the shock velocity is

$$V \equiv \left( \frac{6}{5} \frac{P_s}{\rho_s} \right)^{1/2} = \left( \frac{6}{5} \frac{E'}{4\pi H} \right)^{1/2} \quad (13.13)$$

$$= 7 \times 10^8 \text{ cm s}^{-1}. \quad (13.14)$$

If we assume arbitrarily that this is the correct velocity during the entire 2 s of strong neutrino luminosity, then at the end of this period the shock will be at

$$R_s = 14,000 \text{ km}. \quad (13.15)$$

By this time the shock will almost certainly have caught up with the rarefaction which started when the core collapse first began, so the shock now runs into material of velocity

$$u_1 = 0. \quad (13.16)$$

The shock velocity (13.12) will persist until the shock runs into the boundary between He and H, where it will first accelerate and then decelerate. In the bulk hydrogen,  $H \approx 10^{33}$  g, and

$$U = 3 \times 10^8. \quad (13.17)$$

At  $R_c$  of equation (13.15), the shock pressure is

$$P_c = 3 \times 10^{22}. \quad (13.18)$$

The temperature is now low enough so that positrons no longer are important. Taking therefore just the pure radiation pressure,

$$P_r = 0.46 \times 10^{26} T_{\text{MeV}}^4, \quad (13.19)$$

and correcting for the electrons associated with the matter, we get

$$T = 80 \text{ keV}. \quad (13.20)$$

But the temperature well behind the shock will be substantially higher.

#### 14. OPEN QUESTIONS

1. Why does accretion continue for 2 s, apparently undiminished? Why does it stop then? Assuming vigorous convection in the mantle, it is unclear what fraction of the down stream will accrete, and what fraction will turn around and move back up to the shock front. Tentatively, I assume that stopping accretion means stopping the down stream. Early on, over much of the area of the shock front, the material behind the shock continues the inward motion which it had outside the shock, though with diminished velocity. After the critical time of 2 s, the material behind the shock moves outward over the entire area.

How can one understand qualitatively the amount of material accreted? And how can one estimate the energy emitted in neutrinos per unit mass accreted?

2. Do temperature and density in the region from 100 to 400 km really behave as outlined in § 6? It is there assumed that the down stream in the convective region carries its energy along, with little net work being done on any other material. This seems reasonable as long as the down stream exists and is a continuation of the inward flow of the material coming in from the far outside.

While this is plausible for energy and temperature, it is less clear for the density. With convection, the material velocity relative to the shock front is not necessarily at right angles on the shock surface, and thus the factor of 6 in density is uncertain. Moreover, there may be a gradual decrease in density (at a given  $r$ ) as the shock moves outward. This could decrease the density as compared with that assumed in § 8, and thereby diminish the shock energy.

3. Is the convection correctly described in the two-dimensional calculations by Herant et al. (1992)? In the hydrodynamic theory of turbulence, there is a qualitative difference between two and three dimensions. In three dimensions, large eddies transfer their energy automatically to smaller ones, ending up in Kolmogorov turbulence. In two dimensions this is not the case because of conservation of angular momentum: eddies tend to become larger, as indeed they do in the numerical model of Herant et al.

4. Nucleosynthesis is more complicated in the presence of convection than in the case of pure radial flow. In the latter case, a given material element reaches its highest temperature as it goes through the shock; afterward it cools adiabatically. With convection, the element dives deeply below the shock front before it turns around and joins the up stream. At present, we do not know how deeply it dives, and this determines its maximum temperature, and hence its nucleosynthesis.

Perhaps we may be able to learn something about the details of convection from the observed amount of  $^{56}\text{Ni}$ . Moreover,

Colgate, Herant, & Benz (1992) have emphasized that the  $^{56}\text{Ni}$ , after being produced at small radius, was apparently transported far out into the original He, presumably by convection.

5. Can we now predict the behavior of supernovae of other masses? We have found that the start of the shock (§ 12) depends on the initial density distribution of the star at included mass  $M$ , between 1.5 and  $2 M_{\odot}$ . Does it make any difference whether the progenitor is a red or a blue giant? Is

there an upper limit to the mass of a star which can make a successful supernova?

I am very grateful to Jim Wilson and Ron Mayle for keeping me informed on the progress of their supernova calculations. I wish to thank Stan Woosley for many clarifying discussions, as well as M. E. Herant, W. Benz, and S. A. Colgate for sending me their paper before publication.

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**The Supernova Shock**  
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I had pointed out the importance of convection for the supernova shock in 1990 in an article in *Rev. Modern Phys.* **62**, 801–866. Two-dimensional computations were carried out by Herant *et al.* which yielded successful supernova shocks; they were followed by other authors. 2D computations are probably the best approximation to reality up to now, but they are hard to comprehend. Therefore, in this paper, I make an analytical approximation which simulates the 2D computation quite well. I point out the importance of dissociation energy, of  $\alpha$ -particles into nucleons. The Hugoniot equation must be satisfied at the shock at all times. A large amount of energy must be assembled behind the shock before it can start moving fast.

## THE SUPERNOVA SHOCK

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### ABSTRACT

Vigorous convection is the key to the supernova mechanism. An analytic theory is presented which parallels the computations of Herant et al. Energy is delivered by neutrinos to the convecting medium. The most important quantity is  $\rho_1 r^3$ , where  $\rho_1$  is the density outside the shock. This can be obtained from the computations of Wilson et al., since it is not affected by the convection behind the shock. It is closely related to  $\dot{M}$ , the rate at which matter falls in toward the center. The outgoing shock is dominated by the Hugoniot equation; the shock cannot move out until its energy is of the order of 1 foe ( $= 10^{51}$  ergs). Once it moves, its velocity and energy are calculated as functions of its radius. Nucleosynthesis gives an appreciable contribution to the energy. A substantial fraction of the energy is initially stored as nuclear dissociation energy, and then released as the shock moves out. This energy cannot at present be calculated from first principles, but it can be deduced from the observed energy of SN 1987A of  $1.4 \pm 0.4$  foe. From the result it is shown that about one-half of the infalling material goes into the shock and one-half accretes to the neutron star.

*Subject headings:* shock waves — supernovae: general — supernovae: individual (SN 1987A)

### 1. INTRODUCTION

It is fairly generally agreed that the supernova shock is powered by the neutrinos emitted by the proto-neutron star, a mechanism discovered by J. Wilson in 1982 (Wilson 1985). Unfortunately, numerical computations have given ambiguous results: Wilson & Mayle (1993) have sometimes found a good shock and sometimes not. Other scientists using computers have generally failed. Using an analytic approach, I (Bethe 1993a, hereafter Paper I) found a shock with satisfactory energy of about 1 foe ( $= 10^{51}$  ergs), but the start of the shock remained questionable.

Burrows & Goshy (1993) indicated, by a mathematical argument, that the shock probably cannot get started as long as spherical symmetry is assumed. The same conclusion was reached by Herant et al. (1994, hereafter Paper III) on more physical grounds. Herant et al. use vigorous convection to break spherical symmetry, with satisfactory results.

The idea of convection started from the computations of J. Wilson, R. Bowers, and R. Mayle. These indicated very high entropies,  $S$ , of order  $100 k_B$  nucleon $^{-1}$  and, in part of the star, a strongly negative  $dS/dr$ . On this basis, I suggested (Bethe 1990, hereafter Paper II) that there must be strong convection. This helped to bring neutrino-produced energy to the shock, and to keep the matter around 100–300 km cool, thus reducing the energy loss from electron capture, (see Paper I, § 4).

There are two regions of convection in a Type II supernova, inside and outside the neutrino sphere. The inside convection is driven by a negative gradient in  $Y_e$ , and is responsible for an increase in neutrino emission. This is important because it increases the rate at which energy is delivered to the shock. It is well discussed by Wilson & Mayle (1993).

However, in this paper we shall use the *observed* anti-neutrino flux in SN 1987A. This is the best information we have on neutrino luminosity. But these observations do not have good time resolution. We can get the average luminosity in the first second or two, but no finer detail. To find the luminosity in the first 0.1 s, I assume that it is the same as the average in the first 2 s. This is an underestimate, because, both

from theory and from observation, the luminosity is expected to decrease with time.

The supernova energy is not very sensitive to the neutrino luminosity, as will be discussed in §§ 6 and 7. However, it remains an important theoretical problem to calculate the early neutrino luminosity reliably.

The convection *outside* the neutrino sphere is of prime importance for our theory. It is driven by a negative entropy gradient and has been computed (a) by Herant et al. (1994) and (b) by Miller, Wilson, & Mayle (1993). Unfortunately, they arrive at different conclusions. Herant et al. find that convection gives a powerful engine delivering energy to the shock and that breaking of the spherical symmetry by a two-dimensional computation is essential. Miller et al.'s result from their two-dimensional computation does not differ much from a previous one-dimensional one.

Both calculations are done with great care. The difference lies in the assumptions about the starting conditions. Miller et al. assume that the material out so some radius  $R_1$  is spherically symmetric, and the material outside  $R_1$  has a density fluctuation  $b \sin kx$ , where  $x$  is a coordinate on the surface of the sphere,  $k$  is a wavenumber, and  $b$  is an amplitude. The amplitude  $b$  then increases with time due to convection, and the shock begins to move—the sooner, the bigger  $b$ . Assuming reasonable, i.e., fairly small, values of  $b$ , Miller et al. find that it takes a long time before convection attains a substantial amplitude. It is then too late to revive the stalled shock. In fact, the time is about the same as that at which the shock is revived in the more successful computations of Mayle and Wilson without convection. So it may be understandable why Miller et al. obtained similar results with and without convection.

Herant et al. assume that convection starts already in the prompt shock and spreads from there to the newly infalling material. Benz, Colgate, & Herant (1994) have given arguments for this assumption, and I believe it to be correct (see § 15 of this paper), but there is as yet no actual proof. With this assumption, the shock is started very early, about 0.1 s after “bounce” (see § 6).

## SUPERNOVA SHOCK

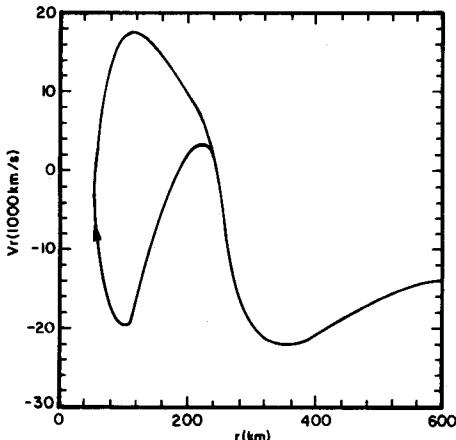


FIG. 1.—Radial velocity, 23 ms after bounce, according to Herant et al. (1994) (Paper III). At  $R < 200$  km, two curves are shown, the fastest inward and fastest outward velocities. The lower curve applies to the cool, infalling material, the upper to the heated material. Actual velocities in the two-dimensional calculation lie between the limits.

Other authors who have worked on this problem include Shimizu, Yamada, & Sato (1993), and Janka & Müller (1993). I shall adopt the Herant theory.

## 2. THE THEORY OF HERANT ET AL.

Herant et al. (1994) have shown in Paper III, by an actual computation, that a revived shock can be started if there is vigorous convection (see also Herant, Benz, & Colgate 1992). I am grateful to M. E. Herant and W. Benz for sending me their manuscript before publication, for showing me their calculations even earlier, and for permitting me to publish Figures 1 and 2 of the present paper, which resulted from their earlier calculations and are not in their published paper (Paper III). They are not responsible for the comments in this section, which are entirely my responsibility.

Figure 1 gives their result for the motion of material, at a time 50 ms after convection starts. There are clearly two streams of material, one going down, the other up, as expected for convection. Figure 2 gives the temperature versus distance  $R$  from the center and shows again the two streams; the lower temperature belongs to the downstream. It starts at about 1

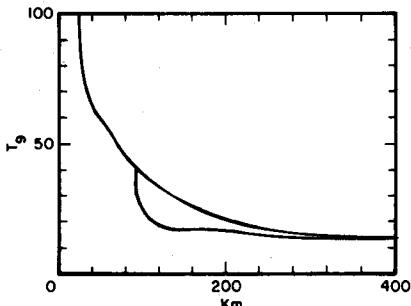


FIG. 2.—Temperature vs.  $R$ , 23 ms after collapse. The lower curve again corresponds to the cool, infalling material and the upper curve to the heated material in the upstream.

MeV at the shock which is located at  $R \approx 400$  km. The material gets slowly heated by neutrinos. At about 100 km, the material, now being hot, tries to move up, which it can only do by first moving sideways and joining the upstream left over from the failed prompt shock. This upstream is on the whole at low velocity but has a strong negative entropy gradient,  $dS/dr < 0$ , and therefore is already in convection.

According to the computation of Herant et al. (hereafter "Herant et al." refers to Paper III), the temperature of the joint upstream starts at 3.4 MeV at 100 km, and then cools adiabatically as it rises. (Interestingly,  $T$  decreases about as  $R^{-1}$ , obeying the theory of Paper I, § 5.) As long as  $T > T_g$ , the material loses energy on balance, while below  $T_g$  it gains energy (slightly); here  $T_g$  is the gain temperature (see Paper I, § 7). It arrives at 400 km with enough energy and pressure to drive a shock.

The material, in a single down-up loop, gains about 4 MeV nucleon $^{-1}$  from neutrino absorption. Herant et al. properly describe it as "a powerful convective heat engine."

When enough energy has been acquired by the convective region, a surprising phenomenon occurs: The shock suddenly moves out with a high velocity, of order  $10^9$  cm s $^{-1}$ . Once this happens, the density decreases and the capacity to absorb neutrinos decreases proportionally; see § 7 of this paper.

Herant et al. have calculated the shock energy after 0.25 s. It is 1.3 and 1.5 foe for stars of initial (main-sequence) mass 15 and  $25 M_\odot$ , respectively, close to the observed energy of  $1.4 \pm 0.4$  foe in SN 1987A, which had a mass of  $18 M_\odot$ . We shall show in § 9 that probably another 0.1 foe is to be added for nucleosynthesis.

In this paper we shall treat the Herant model analytically, and we shall confirm all major points of their theory. In particular, we can explain the sudden breakout of the shock (§ 6).

## 3. SHAPE OF THE SHOCK

The upstream of convection cannot end on the shock. This would mean that matter flows to the shock from outside as well as from inside (i.e., the convection region). This would violate conservation of matter.

So the convection upstream must stay inside the shock front. But also the matter coming in from outside must go to the convection region. To accommodate both, it is necessary for the shock front to be oblique, as indicated in Figure 3. In this figure, the spherical curvature is ignored, so the infalling matter comes in vertically. At the shock, the velocity component parallel to the shock is conserved, but the perpendicular component is reduced by a factor of about 6. Thus the streamlines of the incoming material have a break at the shock, as shown in Figure 3. Thereby they avoid the convecting material.

Figure 4 gives a schematic picture of material motion near the shock. The convecting material is assumed to circulate, as it does in laboratory experiments and in a recent computer simulation of supernova convection by Burrows, Hayes, & Fryxell (1995). The interior of the top of the shock is left void in the figure because I do not know what happens there; but it is just there that convecting material transmits its upward pressure to the shock.

Matter entering from outside the shock dives deep into the convection region and is heated in this process, as described in § 2. When the upstream arrives near the shock, it has more internal energy and more pressure than when it first entered through the shock. At early times, this pressure resists the ram pressure of the infalling material and keeps the shock roughly

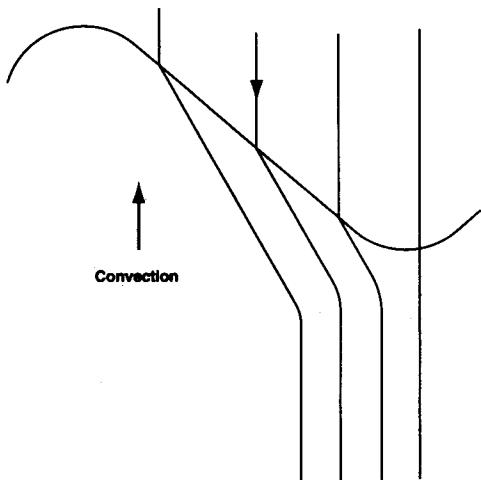


FIG. 3.—Shape of the shock. Material falls in vertically. It must leave room for the hot, convecting material. This is accomplished by having an oblique shock which deflects the incident material to the right.

stationary (details remain to be worked out). This continues for a long time; see § 6. During this time, the upstream material has no place to go but sideways, as indicated in Figure 4: it has to go down again. But, starting from a high temperature, this secondary downstream is probably not useful for absorbing neutrino energy: that function is left to the fresh infalling material which starts out cool.

The material supplied from outside can have two destinations: either it will stay in the convection region, or it may fall further and accrete to the neutron star. The former alternative means that the mass in the convection region increases.

Below the region pictured in Figure 4, some of the fresh material (on the right-hand side of Fig. 4) will be diverted into

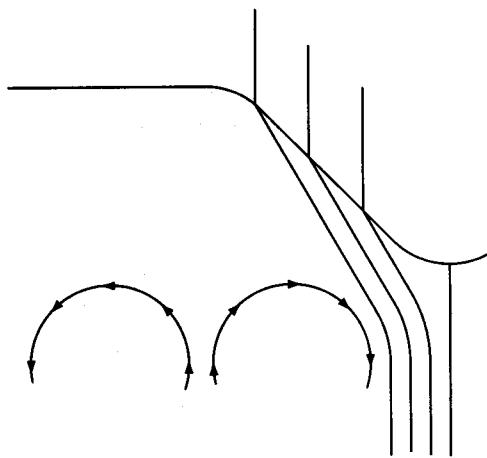


FIG. 4.—A wider view of the shock region. Shown are two semicircles representing the circulating, convecting mass. In the middle of the figure, hot material moves up.

the convection region (center of Fig. 4), adding to the circulating mass. After a while, the pressure of the convecting mass will overcome the ram pressure and drive the shock upward (§§ 6 and 7).

As already mentioned, probably only the fresh matter entering through the shock can absorb neutrinos effectively because only it starts out cool. The upstream is hot, and therefore the electron capture is likely to cancel, pretty nearly, the energy gain from neutrino capture. Therefore, only the neutrinos which hit the cool primary downstream will be effective in giving energy to the convection region. We call  $\eta$  the fraction of neutrinos that are effective. This fraction  $\eta$  is calculated in Appendix A and is found to be about  $\frac{1}{3}$ .

On the other hand, the downstream will not go precisely vertically down but may be oblique or curved; this will increase its solid angle. The final result for the energy is not very sensitive to  $\eta$ , as shown in §§ 6 and 7.

The net heating is the difference between the heating by neutrinos and the cooling by electron capture. The latter is proportional to  $T^6$  (Paper I, eq. [4.1]). In Paper I, I defined the gain radius  $R_g$  as the place where cooling and heating balance. The vigorous convection of Herant et al. has the advantage that the original downstream, coming down from the shock, is cool; hence the gain radius  $R_g$  will be smaller than for spherical symmetry, and therefore the neutrino flux will be greater, a fact exploited by Herant et al. Somewhat arbitrarily, we assume  $R_g$  to be 120 km.

In the upstream, the neutrino heating is assumed to compensate for the cooling by electron capture.

#### 4. DENSITY

The density outside the shock can be obtained from one-dimensional computer calculations. We take, in particular, the computation by Wilson and Mayle of 1989 November 27 (Wilson & Mayle 1989) of a star of initial mass  $18 M_\odot$ . These results agree well with the two-dimensional computations of Herant et al. It will be convenient to approximate them by simple algebraic formulae, as follows:

$$\begin{aligned} \rho_1 R^3 &= 0.45 R_s \times 10^{31} && \text{for } 3 < R_s < 5, \\ \rho_1 R^3 &= 2.25 \times 10^{31} && \text{for } 5 < R_s < 20, \\ \rho_1 R^3 &= 0.12 R_s \times 10^{31} && \text{for } 20 < R_s. \end{aligned} \quad (4.1)$$

These formulae approximate the computed result within about 10%. We have assumed that the density at a given  $R$  stays reasonably constant during the short time (about 0.1 s) of shock acceleration by neutrinos.

We assume that the density increases by a factor of 6 at the shock. This is between the factor of 7 valid if the particles behind the shock are relativistic (photons or electrons), and the factor of 4 for nonrelativistic free particles (nucleons or heavier nuclei). In the computed shock, partial pressure from relativistic particles is usually greater than that from nonrelativistic ones, therefore we choose a factor closer to the relativistic 7.

If the shock radius  $R_s$  is greater than 300 km, we take the density to be that just inside the shock radius  $R_s$ . This is very conservative; usually the density increases as  $r$  decreases. But the computations by Herant et al. at their largest value of  $R_s$ , 3000 km, show only a moderate increase of density between 3000 and 300 km, maybe as  $r^{-1/2}$ . From 300 km down to the gain radius, we assume the density to increase as  $R^{-(3-\eta)}$ . The two-dimensional computations by Herant et al. indicate that

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the exponent of  $R$  changes from 2.7 to 25 ms after bounce to 2.3 at 50 ms, so  $n$  increases from 0.3 to 0.7.

As will be shown in equation (5.6), the fraction of neutrino energy absorbed is proportional to

$$I = \int_{R_s}^{R_a} \rho_2 dr, \quad (4.2)$$

where  $R_g$  is the gain radius (see Paper I, § 7), and  $R_a$  is the radius at which half the material is nucleons and half  $\alpha$ -particles; following Paper I, § 6, we take this to be 300 km. Then

$$I = \rho_2(R_s) R_a [(R_a/R_s)^{2-n} - 1]/(2-n). \quad (4.3)$$

We take  $R_s = 120$  km and  $n = 0.5$ . Using equations (4.1),

$$\rho_1(R_s) = 5 \times 10^8, \quad (4.4)$$

$$I_1 = 3 \times 10^9 \times 3 \times 10^7 \times 1.97 = 1.8 \times 10^{17}. \quad (4.5)$$

This, however, holds only when the shock is at  $R_s$ . When the shock moves out to  $R_a$ , I assume that the density at  $R_a$  equals the density at the shock (see above), and take the latter to be  $6\rho_1(R_s)$ . Then

$$I = I_1 \frac{\rho_1(R_s)}{\rho_1(R_a)}. \quad (4.6)$$

The density in the important region between gain radius and  $\alpha$ -radius tends to be higher in the calculations by Herant et al. than in the calculations without convection. This can be seen by comparing the dependence on  $r$ . For instance, the 1989 November 27 computation by Wilson & Mayle (1989) at time 0.6 s postbounce, the density between 100 and 300 km varies about as  $1/r$ , whereas in the Herant calculation it behaves as  $r^{-2.5}$ ; see the paragraph above equation (4.2). Since the density at the larger  $r$  is fixed by the density at the shock (which is the same in both cases), the Herant densities on the average are higher, and I am simulating these.

I attribute this result to a fundamental difference due to convection. In conventional computations, a given mass element crosses the region of effective neutrino absorption only once, going down. In convection, there is circulation in the convection region, and much of the incoming matter accumulates in this region. Therefore, for a given rate of mass infall from the outside, the density in the convective region will be substantially greater than in the conventional computation. Since neutrino absorption is proportional to matter density, the energy given by the neutrinos to the matter will be greater in convection.

## 5. NEUTRINO HEATING

The absorption of neutrino energy by matter is

$$\dot{E} = K\eta \int \frac{L}{4\pi r^2} 4\pi \rho r^2 dr X, \quad (5.1)$$

where  $L$  is the neutrino luminosity of the neutron star in ergs  $s^{-1}$ .  $K$  is the opacity,

$$K = \frac{1}{2} N_A \sigma, \quad (5.2)$$

where  $N_A$  is Avogadro's number and  $\sigma$  is the cross section for capture of a neutrino (antineutrino) by a neutron (proton),

$$\sigma = 0.9 \times 10^{-43} e^2 \text{ cm}^2, \quad (5.3)$$

where  $e$  is the neutrino energy in MeV. The average of  $e^2$  can be found using the observation of neutrinos from SN 1987A,

$$\langle e^2 \rangle = 250 \text{ MeV}^2; \quad (5.4)$$

the computations of Wilson & Mayle (1989) are in good agreement with this. Then

$$K = 0.7 \times 10^{-17} \text{ cm}^2 \text{ g}^{-1}. \quad (5.5)$$

The factor  $X$  in equation (5.1) is the mass fraction of free nucleons in the nuclear component.  ${}^4\text{He}$  nuclei can capture only neutrinos of very high energy ( $\geq 20$  MeV), which are very rare in the spectrum of neutrinos from the neutron star; even for these, the cross section is a small fraction of equation (5.3).

In Paper I (eq. [6.5]) I showed that in the initial collapse,  $X = \frac{1}{2}$  occurs at  $R_a = 300$  km. I shall use the approximation  $X = 1$  for  $r < R_a$ ,  $X = 0$  for  $r > R_a$ . This approximation is used because there are at present no reliable data on  $\rho$  and  $X$  beyond 300 km. If we assume  $L$  to be independent of  $r$  (this will be corrected below eq. [5.7]), equation (5.1) reduces to

$$\dot{E}/L\eta \equiv \alpha = K \int_{R_s}^{R_a} \rho_2 dr, \quad (5.6)$$

where  $R_g$  is the gain radius (see § 3) and  $\alpha$ , defined by equation (5.6), is the utilization factor for the neutrino energy. The interval from  $R_s$  to  $R_a$  is assumed to be inside the shock, hence the density is  $\rho_2$ . (If  $R_s < R_a$ , the upper limit of the integral should be  $R_s$ , where  $R_s$  is the shock radius.)

The integral in equation (5.6) has been calculated in § 4. In particular, if the shock is at  $R_a$ , it is

$$I_1 = 1.8 \times 10^{17}. \quad (4.5)$$

Hence the optical depth of the convective region, using equations (5.5) and (5.6), is

$$\alpha_1 = K I_1 = 1.2. \quad (5.7)$$

This is very large, hence the luminosity will actually decrease exponentially in the region in question. Taking this into account, the fraction of neutrino energy transferred to matter is

$$\dot{E}/L\eta = 1 - e^{-\alpha_1} = 0.7. \quad (5.8)$$

This is enormous: none of us, three years ago, would have believed that 70% of the neutrino energy could be transferred to the shock. Herant et al., in their computer calculation, find a similar result.

The neutrino luminosity in SN 1987A was (for the first 2 s)

$$L = 28 \text{ foe s}^{-1}. \quad (5.9)$$

Thus, setting  $\eta = \frac{1}{3}$ , the energy given to the shock (while the shock front is at 300 km) is

$$\dot{E} = 6 \text{ foe s}^{-1}. \quad (5.10)$$

The difference between  $\alpha$  and  $1 - e^{-\alpha}$  is due to the absorption of neutrinos in the relevant region. In § 7, when we discuss the moving shock, we shall not take this into account explicitly; instead, we shall assume that the rate of energy increase is reduced in the same ratio as the density at  $R_a$ , similar to equation (4.6); then

$$\frac{dE}{dt} = 6 \text{ foe s}^{-1} \frac{\rho_1(R_s)}{\rho_1(R_a)}. \quad (5.11)$$

The densities are given by equation (4.1).

## 6. VIRIAL THEOREM

The virial theorem relates quantities inside and on the surface of the shocked region:

$$\int_g^s \left( 3P - \frac{GM_r}{r} \rho \right) r^2 dr = (PR^3)_s - (PR^3)_g . \quad (6.1)$$

Here  $P$  is the pressure, the subscript  $s$  refers to the shock, and  $g$  refers to the gain radius.  $GM_r/r$  enters as  $r$  times the gravitational force; it happens to be also the gravitational potential due to the material inside  $r$ , omitting the (usually small) potential due to material outside  $r$ .

We consider shock radii  $R_s \leq 300$  km; then the nuclear material is mostly dissociated into nucleons, and the temperature  $T > 1$  MeV. Then the electron-positron gas may be treated together with electromagnetic radiation, giving a radiation pressure

$$P_r = 1.25 \times 10^{26} T^4 , \quad (6.2)$$

where the temperature  $T$  is in MeV. This  $P_r$  is in general small compared to the material pressure

$$P_m = 0.96 \times 10^{18} \rho T . \quad (6.3)$$

The pressure  $P$  on the left-hand side of equation (6.1) is related to the energy; we have

$$3P_r = w_r , \quad (6.4)$$

where  $w_r$  is the radiation energy per unit volume. Further,

$$3P_m/2\rho + d - GM_r/r = \varepsilon_m \quad (6.5)$$

is the material energy per unit mass (excluding any kinetic energy). Here  $d$  is the dissociation energy per unit mass; we choose  $^{16}\text{O}$  as the standard. (The material which forms the bulk of the shock is mostly  $^{16}\text{O}$  in the presupernova; see also § 9.) Then we have

$$\int [w_r + (\varepsilon_m + 3P_m/2\rho - d)\rho] r^2 dr = (PR^3)_s - (PR^3)_g . \quad (6.6)$$

We note that

$$\varepsilon_m + \varepsilon_m \rho = w , \quad (6.7)$$

is the total energy per unit volume, and we set

$$d - 3P_m/2\rho = d' , \quad (6.8)$$

$$D = 4\pi \int d' \rho r^2 dr = d'_A M_s , \quad (6.9)$$

where  $M_s$  is the mass of the shocked material. Then equation (6.7) becomes

$$E - D = 4\pi(PR^3)_s - 4\pi(PR^3)_g \equiv A - X , \quad (6.10)$$

where  $E$  is the total energy (excluding kinetic) in the shock.

The term  $A$  may be evaluated; the pressure behind the shock is given by the Hugoniot equation

$$P_s = (5/6)\rho_1(U + v)^2 , \quad (6.11)$$

where  $\rho_1$  is the density just outside the shock,  $U$  is the velocity of the shock, and  $v$  is the infall velocity of the material outside the shock. The factor  $5/6$  is related to our assumption that the density increases by a factor of 6 in the shock. A strong shock

has been assumed, i.e.,

$$P_1 \ll P_s , \quad (6.12)$$

where  $P_1$  is the pressure just outside the shock. The quantity  $\rho_1 R_g^2$  which enters equation (6.10) is given in equation (4.1). The velocity of infall  $v$  can be obtained from the computations of Wilson & Mayle (1989); it is

$$v_9 = 5.8/r_7 + 0.1 . \quad (6.13)$$

It is important that  $v$  and  $\rho_1$  refer entirely to conditions outside the shock; since the shock is supersonic, these conditions are not affected by events behind the shock, such as whether there is convection or not. This justifies taking the results from the one-dimensional computations of Wilson & Mayle.

In order for the shock to get started, we must have  $U \geq 0$ . Clearly,  $U = 0$  gives a minimum value  $P_s$ , hence to  $A$ , and therefore to the required energy  $E$  (eq. [6.10]); we call this  $E_0$ . We shall calculate  $A$  for  $R_s = 300$  km, this being the point where half the nuclear material is  $\alpha$ -particles and half nucleons (see Paper I, § 6), before heating by neutrinos; we call this  $R_\alpha$  and have

$$A(R_\alpha) = 4\pi(PR^3)_\alpha = (10\pi/3)\rho_1 R_\alpha^3 v^2 \\ = 10.5 \times 1.35 \times 10^{31} \times 4.2 \times 10^{18} = 0.58 \text{ foe} . \quad (6.14)$$

The term  $X$  in equation (6.10) is more difficult to evaluate. In Paper I, equation (12.8), we found

$$X = 4\pi P_g R_g^3 = 0.08 \text{ foe} , \quad (6.15)$$

a very small value. On the other hand, we can argue that between  $R_\alpha$  and  $R_s$  the density should go roughly as  $r^{-2}$ , the temperature as  $r^{-4}$ ; hence the material pressure  $P_m \sim \rho T \sim r^{-3}$  (the radiation pressure is small by comparison). Then

$$X \approx A = 0.58 \text{ foe} . \quad (6.16)$$

A more detailed calculation will be needed to determine  $X$ ; we leave it as  $X$  in the following. But we assume  $X$  to remain unchanged as the shock propagates. Then the initial values (at the time the shock starts) of  $E$  and  $D$  are related by equation (6.10); thus

$$E_0 - D_0 = A - X . \quad (6.17)$$

$A - X$  is either zero or not very large; thus nearly all the energy of the shock is initially tied up in dissociation.

As the shock moves outward, the temperature, at least in the front part, will fall. This will make nucleons recombine, hence the dissociation energy  $D$  will decrease. Thus, even if the energy  $E$  remains at  $E_0$ ,  $E - D$  will increase, and since we assumed that  $X$  stays constant,  $A$  will increase, and so, according to equation (6.11), will  $U + v$ ; thus  $U > 0$  and the shock will move out farther. This will be discussed in § 7. Thus dissociation is a convenient way to store energy so that it can easily be recovered. When the shock is at large distance  $R_s$ , there is no dissociation.

I have not found a way to calculate the shock energy  $E$ . But I shall use the observed shock energy in SN 1987A to obtain the dissociation energy  $D_0$  at the time shock starts moving. In order to do this, I must calculate the amounts of energy which are added or subtracted from  $E_0$  as the shock moves out.

I have assumed in equation (6.14) that the shock is stationary at 300 km. This is reasonable because the prompt shock proceeds to about 200 km before it dies. It provides a floor for the accretion shock which we are dealing with in this section.

To determine how  $A$  depends on the shock position, I assume that the top equation (4.1) continues to hold for  $R_7 < 3$ . The infall velocity cannot easily continue to increase as fast as indicated in equation (6.14); it is more reasonable to assume that between 300 km and the actual shock position,

$$v \sim R^{-1/2}, \quad (6.18)$$

i.e., that  $v$  remains a constant fraction of the free-fall velocity. Then in equation (6.14) the factor  $\rho_1 R_s^3$  goes as  $R_s$ , the factor  $v^2$  as  $R_s^{-1}$ ; hence  $A$  is independent of  $R_s$ , for  $R_s < 3$ .

How does the shock behave before it has acquired the energy  $E_0$ ? We start from the prompt shock. After its stalls, it may recede for some time, as Wilson and collaborators have shown. This is due to the ram pressure of the infalling material. But it cannot recede to very small  $R$  because on the inside we have very high density and pressure. Hence, for some time, the shock is almost stationary. Its actual location can only be determined by numerical computation. In fact, it is not well defined, due to the two-dimensional convection.

It is confusing that the shock can be stationary for two entirely different reasons. In the situation just described (situation I), its position is due to a balance between two strong opposing forces, the internal and the ram pressure. No neutrino energy has yet been supplied. The specific energy (total energy per unit mass [epm]) is negative because it includes a very large negative component, the gravitational potential energy. Because the epm is negative, the material inside the shock cannot escape from the star, let alone propel a shock outward.

Situation II is the one described by  $E_0$ : Neutrino energy has now been supplied, and epm has become positive. The internal pressure is now provided by temperature rather than density, in fact the density is moderate, of order  $10^{10}$  if the shock is located at 300 km. Since epm  $> 0$ , the material can drive the shock outward.

The problem is how to go from situation I to situation II. That this can be done is shown by the calculations of Herant et al. Here deviation from spherical symmetry is necessary.<sup>1</sup> But the details need further investigation, probably a two-dimensional computation including a careful study of the distribution of the epm in the convecting region and of the degree of involvement of the material from the dying prompt shock. It should also be determined whether the shock surface at 300 km still deviates strongly from a sphere.

The transition from the first to the second type of stationary shock is the crucial step in the supernova. Equation (6.17) merely indicates where this transition has to end. In § 12, after evaluating  $D_0$ , we shall discuss how the necessary energy is supplied. We shall show that it takes about 0.2 s to supply the energy to get the shock moving.

It is interesting that  $A$  in equation (6.14), and hence the minimum shock energy,  $E_0$ , appears to be independent of the rate at which energy is delivered by neutrinos. This is surprising because in previous calculations the rate of energy supply was all-important. For instance, the Livermore group found that varying  $\dot{E}$  by roughly 10% varied the final supernova energy by roughly 50%. As a matter of fact (§ 13), also in our case, it turns out that for any rate of mass infall  $\dot{M}$ , a

<sup>1</sup> In some computations of the Livermore group, a propagating shock was achieved without deviation from spherical symmetry, but the final energy always stayed low, about 0.5 foe.

minimum rate  $\dot{E}$  of energy supply is required, and hence a minimum neutrino luminosity  $L$ .

The important result of this section is that the shock must acquire a large energy  $E_0$  before it can start moving.

## 7. THE RUNNING SHOCK

The motion of the shock is governed by the Hugoniot equation (6.11). Suppose the energy  $E$  of the shock has been calculated at some shock radius  $R_s$ . The quantity  $\rho_1 R_s^3$  can be read from equation (4.1), which, as will be remembered, are derived from the infall computations of Wilson & Mayle (1989). Then, from equations (6.10) and (6.11), we can calculate  $U + v$ . The velocity of the infalling material is given in equation (6.13). Thus we obtain the shock velocity  $U$ , and hence the time  $\Delta t$  required to go to the next shock position  $R_s + \Delta R$ .

The main feature in the running shock is the recombination of nucleons into  $\alpha$ -particles. This reduces the dissociation energy  $D$  and, assuming the total energy  $E$  to be constant, increases

$$A \equiv 4\pi P_s R_s^3 = E - D + X. \quad (7.1)$$

A proper treatment would require a computer calculation, paying close attention to recombination; a one-dimensional computation should be sufficient. Here we shall be content with a schematic model.

When the material consists entirely of  $\alpha$ -particles, the effective dissociation energy  $d'$  per particle is zero; that is (cf. § 12),

Dissociation of  $^{16}\text{O}$  into  $^4\text{He} - (3/2)T$  (temperature 600 keV)

$$\begin{aligned} &= 0.9 \text{ MeV nucleon}^{-1} - 0.9 \text{ MeV nucleon}^{-1} \quad (7.2) \\ &= 0. \end{aligned}$$

We assume that the recombination of nucleons into  $\alpha$ -particles takes place between  $R = 300$  and  $R = 800$  km, at a uniform rate. We take the value of  $D$  at 300 km to be 1.0 foe (see eq. [12.5]). For the calculation outlined in the first paragraph of this section, we assume that  $E$  changes little by comparison with  $D$ . Then  $A$  in equation (6.2) will increase from 0.58 to 1.58 fo as  $R_s$  changes from 3 to 8; we assume it to stay constant thereafter.

The rate of energy increase is given by equation (5.11). According to equations (4.1), in the most important interval, 300–500 km,

$$\frac{\rho_1(R_s)}{\rho_1(R_s)} = \left( \frac{R_{88}}{R_{38}} \right)^2 = \frac{0.3^2}{R_{38}^2}. \quad (7.3)$$

hence

$$\frac{dE}{dt} = \frac{0.5}{R_{38}^2} \text{ foe s}^{-1}. \quad (7.4)$$

Thus the integration is straightforward. The increase of energy in the running shock is

$$\Delta E = 0.23 \text{ foe}, \quad (7.5)$$

a rather small increase.

Figure 5 shows the energy  $E$  as a function of shock radius. Nearly all the energy has already been acquired when the shock is at 500 km. This is because the density decreases rapidly for  $R_s > 500$  (see eq. [4.1]).

Figure 5 also shows the velocity  $U$  of the shock versus its radius, in units of  $10^9 \text{ cm s}^{-1}$ . Up to  $R_s = 500$  km, this velocity

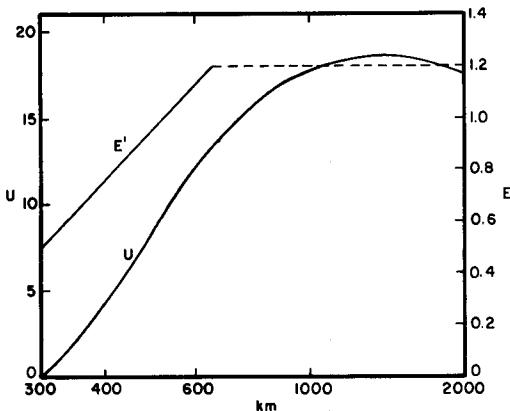


FIG. 5.—The moving shock. Curve U shows the shock velocity as a function of shock radius  $R$ ;  $U$  is in units of  $10^9 \text{ cm s}^{-1}$ . Curve  $E'$  gives the energy in the shock, in foe. Both curves are schematic only.

remains less than  $10,000 \text{ km s}^{-1}$ . This is less than in most previous computations. The reason for the relatively small velocity is the large velocity  $v$  of the infalling material. Only for  $R > 500 \text{ km}$  does the infall velocity decrease rapidly; then the shock velocity increases (Fig. 5).

The time required to get to  $100 \text{ km}$  is

$$t_2 = 0.08 \text{ s}. \quad (7.6)$$

This is after the  $t_1 = 0.20 \text{ s}$  during which the shock is essentially at rest at  $300 \text{ km}$ . Beyond  $1000 \text{ km}$ , the shock acquires still more energy from nucleosynthesis (§ 9). Using Woosley's unperturbed

$$\rho_1 R^3 = 6 \times 10^{31}, \quad (7.7)$$

this gives a shock velocity of about

$$U_{\text{final}} = 13,000 \text{ km s}^{-1}. \quad (7.8)$$

This high velocity, and the long time (about 2 s) between the end of shock acceleration and the drop of neutrino luminosity strengthens my argument (Bethe 1993b) that the shock will persist after that drop in luminosity, rather than fall back by gravity.

The shock velocity decreases when the shock enters the hydrogen region of the progenitor, then increases again near the star surface. These changes occur long after the shock has acquired its full energy; in fact, its energy decreases somewhat because it has to pick up material of negative potential energy (§ 10).

The important result of this section is that the shock acquires only a modest amount of energy while running. This result had already been obtained by Herant et al.

#### 8. ELECTRON SCATTERING

Neutrinos can give energy also to electrons, positive or negative, by elastic scattering. Since the energy of an individual neutrino is much greater than of an individual electron, about half the neutrino energy is transferred. The cross section for this process has been calculated by Tubbs & Schramm (1975) and simplified for our conditions in Paper I, equation (10.1). The efficiency of energy transfer, according to Paper I, equa-

tion (10.5), is

$$\alpha_e = 2.0 \times 10^{-11} \int T^4 dr, \quad (8.1)$$

where  $T$  is the electron temperature in MeV. Of course, this expression is independent of material density.

I use the temperature distribution in Paper I § 5, which is based on hydrostatic equilibrium behind the shock. Then I find, for the efficiency of transfer of neutrino energy to electrons,

$$\alpha_e = 2.0 \times 10^{-4} \int T^4 dr, = 0.13\%. \quad (8.2)$$

In contrast to the transfer to nucleons, this should be essentially independent of time (Paper I, §§ 5 and 6), and therefore proportional to the integrated neutrino luminosity (see eq. [5.9]),

$$\int_0^2 L dt = 56 \text{ foe}. \quad (8.3)$$

To this we should add the contribution of  $\mu$ - and  $\tau$ -neutrinos. From the computer calculations of Wilson & Mayle (1989), it is believed that each of these species has an intensity  $\int L dt$  about equal to that of  $\nu_e$ . But the cross section is only about one-sixth of that of electron neutrinos; on the other hand, the individual neutrino energy is somewhat higher than for  $\nu_e$ . Thus we assume (see Paper I, below eq. [10.6]) that the contribution of  $\nu_\mu + \nu_\tau$  is about 50% of that of  $\nu_e$ ; then the total energy from electron collisions is

$$E_3 = 56 \times 1.5 \times 1.3 \times 10^{-3} = 0.11 \text{ foe}. \quad (8.4)$$

This is independent of  $\dot{M}$ .

The contribution from equation (8.4) may have been overestimated. The temperature  $T$  at small  $r$  (100–300 km) at early times is mostly determined by the nuclear component (Paper I, § 6). At later times (0.1–1 s) when the density has dropped,  $T$  may also drop.

#### 9. NUCLEOSYNTHESIS

We know from optical measurements that in SN 1987A copious  $^{56}\text{Ni}$  was formed, namely,

$$M(^{56}\text{Ni}) = 1.5 \times 10^{32} \text{ g}. \quad (9.1)$$

It is commonly assumed that the formation of Si + S is about 3 times that of Ni; thus

$$M(\text{Si} + \text{S}) = 4.5 \times 10^{32} \text{ g}. \quad (9.2)$$

According to Woosley's calculation of the progenitor of SN 1987A, the material which becomes the supernova shock was originally half  $^{16}\text{O}$  and half Si + S. Hence the energy set free in nucleosynthesis is

$$\begin{aligned} 0.53 \text{ MeV nucleon}^{-1} &\text{ for formation of } ^{56}\text{Ni}, \\ 0.22 \text{ MeV nucleon}^{-1} &\text{ for formation of } ^{28}\text{Si} + ^{32}\text{S}. \end{aligned} \quad (9.3)$$

Thus the total energy from nucleosynthesis is

$$\begin{aligned} \text{From } ^{56}\text{Ni}, & 0.08 \text{ foe}, \\ \text{From Si} + \text{S}, & 0.10 \text{ foe}, \end{aligned} \quad (9.4)$$

or 0.18 foe.

The location of nucleosynthesis is calculated in Appendix C.

## 10. BINDING ENERGY OF THE EJECTA

The considerations of §§ 6–9 follow the energy of the shock out to about 5000 km. But before it can emerge, the shock has to pick up the envelope of the star, and this has a considerable binding energy in the gravitational potential. This can be calculated from the presupernova distribution of density.

The potential energy in the gravitational field is  $-V_g$ , where

$$V_g = \int_{M_1}^{M_2} \frac{GM_r}{r} dM_r; \quad (10.1)$$

$M_r$  is the mass included in the sphere  $r$ , and  $dM_r = 4\pi\rho(r)r^2 dr$ .  $M_1$  is the mass of the compact object remaining after the supernova,  $M_1 \approx 1.73 M_\odot$ , and  $M_2$  is the mass of the progenitor, which does not matter much because  $GM/r$  is very small. From Woosley's presupernova computations, I find for SN 1987A

$$V_g = 1.3 \text{ foe}. \quad (10.2)$$

The gravitational energy is partly compensated by the internal (thermal) energy. For this, the virial theorem is useful:

$$3 \int (P/\rho)dM_r = V_g - 4\pi P_1 R_1^3. \quad (10.3)$$

$P_1$  and  $R_1$  are pressure and radius at  $M_1$ . From the 1989 November 27 computation by Wilson & Mayle (1989), at time 0.01 s after "bounce,"

$$\Pi = 4\pi P_1 R_1^3 = 0.08 \text{ foe}. \quad (10.4)$$

The computation of Wilson & Mayle at this early time reflects the Woosley presupernova calculation.

The energy per unit mass in the envelope (where there is no dissociation) is

$$\begin{aligned} \varepsilon &= 3P/\rho \quad \text{for radiative energy}, \\ \varepsilon &= 3P/2\rho \quad \text{for material (nonrelativistic) energy}. \end{aligned} \quad (10.5)$$

In the region between  $M_r = 2$  and  $3 M_\odot$ , the fraction of radiative pressure is fairly constant at 46%. Assuming this to hold generally, the total energy, thermal and gravitational, is

$$-B = (0.54/2 + 0.46)(V - \Pi) - V, \quad (10.6)$$

$$B = 0.27V + 0.73\Pi = 0.42 \text{ foe}. \quad (10.7)$$

This is the binding energy of the ejecta in the presupernova stage of SN 1987A.

## 11. THE SUPERNOVA ENERGY

The corrections  $C$  to the energy  $E_0$  are now

- From the running shock , 0.23 foe ,
- From collisions with electrons , 0.11 foe , (11.1a)
- From nucleosynthesis , 0.18 foe ,

or 0.52 foe. From this must be subtracted the binding energy of the ejecta  $B = 0.43$  foe; thus

$$C = 0.52 \text{ foe} - 0.43 \text{ foe} \approx 0.1 \text{ foe}. \quad (11.1b)$$

So the final energy is

$$E_f = E_0 + C. \quad (11.2)$$

The observed energy in SN 1987A is (Bethe & Pizzichero 1990)

$$E_{\text{obs}} = 1.4 \pm 0.4 \text{ foe}. \quad (11.3)$$

Hence the initial energy (at the start of the shock) is

$$E_0 = 1.3 \pm 0.4 \text{ foe}. \quad (11.4)$$

## 12. DISSOCIATION ENERGY

At the time the shock gets started (§ 6), we assume that all of the material behind it is nucleons. Hence the dissociation energy per nucleon is, starting from  $^{16}\text{O}$ ,

Full dissociation into  $\alpha$ -particles , 0.9 MeV ,

Dissociation of  $\alpha$ -particle into nucleons , 7.0 MeV ,

or 7.9 MeV. From this we have to subtract  $3P_m/2\rho$ , which occurs in the virial theorem;  $P_m/\rho = T$ , the temperature. We take the average temperature to be 2 MeV, so  $(3/2)T = 3.0$  MeV, and we have

Effective dissociation energy,

$$d' = 4.9 \text{ MeV nucleon}^{-1}. \quad (12.1)$$

This is equivalent to  $4.7 \times 10^{18} \text{ ergs g}^{-1}$ .

From equation (6.17),

$$D_0 = E_0 - A + X. \quad (12.2)$$

Inserting  $E_0 = 1.3 \pm 0.4$  and  $A = 0.58$ , we find

$$D_0 = 0.7 \text{ foe} + X \pm 0.4; \quad (12.3)$$

with (cf. eqs. [6.15] and [6.16]),

$$0.07 \text{ foe} < X < 0.58 \text{ foe}; \quad (12.4)$$

thus

$$D_0 = 1.0 \pm 0.6 \text{ foe}, \quad (12.5)$$

a result with unfortunately wide limits. Dividing by the specific dissociation energy (eq. [12.1]), we get the mass in the shocked material:

$$M_s = (2.1 \pm 1.3) \times 10^{32} \text{ g}. \quad (12.6)$$

The energy in the starting shock is

$$E_0 = 1.3 \pm 0.4 \text{ foe}. \quad (12.7)$$

The rate of energy supply, according to equation (5.10), is

$$6 \text{ foe s}^{-1}. \quad (12.8)$$

Hence the time required before the start of the shock is

$$t_1 = 0.22 \pm 0.07 \text{ s}. \quad (12.9)$$

During this time, according to the computation of Wilson & Mayle (1989), the amount of material falling in toward the center is

$$M_{\text{in}} \approx 4 \times 10^{32} \text{ g}. \quad (12.10)$$

Comparing with equation (12.6), about  $50\% \pm 30\%$  of the infalling material goes into the shock; the rest accretes to the proto-neutron star.

Thus, in a roundabout way, we have obtained an estimate of the partition of the infalling material between accretion and shock. It is very rough, but it shows that at least some of the material must go into the shock, indicating convection, and some will accrete as is necessary to obtain sufficient mass for the proto-neutron star. Of course, the partition between shock and accretion is actually determined by hydrodynamics; to calculate the hydrodynamics remains a problem.

The time of 0.2 s is shorter than that in successful one-dimensional calculations (about 0.5 s) but longer than in the calculations of Herant et al. ( $< 0.1$  s). The latter difference may

be due partly to the fact that none of Herant's infalling material accretes and partly to their higher neutrino luminosity.

### 13. MINIMUM LUMINOSITY

To get the shock started, equation (6.17) must be fulfilled:

$$E_0 - D_0 = A - X. \quad (6.17)$$

At a given time  $t$ , after bounce,

$$E_0 = \dot{E}t_1, \quad (13.1)$$

and

$$D_0 = M(t_1)\beta d', \quad (13.2)$$

where  $d'$  is the dissociation energy per unit mass, given in equation (12.1);  $\beta$  is the fraction of the infalling mass going into the shock (discussed below eq. [12.10]); and  $M(t_1)$  is the amount of matter fallen in by time  $t_1$ . The right-hand side of equation (6.17) is presumably positive, so the equation can only be fulfilled if  $\dot{E}$  is sufficiently big.  $\dot{E}$  in turn (see § 5) is proportional to the neutrino luminosity  $L$ , so we find that

$$L > L_{\min}. \quad (13.3)$$

The supernova can only work if the neutrino luminosity is above a certain minimum, similar to the conclusion of Wilson & Mayle and other authors.

It is not easy to determine  $L_{\min}$ . It is helpful for the supernova mechanism that the amount of matter infalling,  $M(t_1)$ , increases less than linearly with  $t_1$ , while  $E_0$  increases linearly (assuming  $L$  constant). So there is a good chance that equation (6.17) can be fulfilled for larger  $t_1$ , even if it cannot be for small  $t_1$ . But obviously, a long delay  $t_1$  from bounce to shock is a complicated situation. It seems that  $L = 30 \text{ foe s}^{-1}$  is sufficient, but it is not clear how much lower  $L$  is permitted to be.

### 14. ACCRETION

Some of the material falling in from the outside will accrete to the proto-neutron star. We might have hoped that the amount of this could be obtained from two-dimensional computations, but there is no sign of it in the work of Herant et al.

The convection loops which dive deep into the star (100 km) have a horizontal leg which adjoins the nonconvecting atmosphere of the neutron star. I suggest that some of the matter in the convective loop "rubs off" by Kelvin-Helmholtz instability and thereby falls to smaller  $r$ . They are then inside the gain radius (Paper I § 4), so they suffer a net loss of energy and thereby fall into the proto-neutron star.

Herant et al. state that they get too little accretion. The mechanism discussed in the last paragraph should help. But it is a delicate question how much accretion is "right." It would be wrong to call this accretion "fallback" because the material comes originally from the far outside. The calculation in § 12 is at present the only estimate of accretion known to me.

Accretion is important not only for determining the mass of the proto-neutron star, but also in connection with neutrino luminosity. In Paper I (Fig. 1) is shown the neutrino luminosity of SN 1987A as observed by Kamiokande and IMB, as a function of time. It shows a distinct break at about 2 s, from about 20 to 3  $\text{foe s}^{-1}$ . An attractive interpretation is that for the first 2 s the neutrinos come from accretion; the accreting material loses its energy when hitting the proto-neutron star, and this energy is carried away by neutrinos. But this would mean that accretion continues for 2 s, which is not compatible with our theory.

### 15. START OF CONVECTION

Benz et al. (1994) point out that convection due to negative entropy gradient starts in the stalling prompt shock and from there spreads to the infalling material. This in fact is clearly shown in the numerical computations of Herant et al. (1994).

That the dying shock is likely to have convection had already been pointed out by Cooperstein, Bethe, & Brown (1984), but they were unable to find any beneficial effect on the shock arising from that convection. This could be found only after the intrinsically two- (or three-) dimensional character of the convection was realized.

Convection in the dying shock probably starts from the Richtmyer-Meshkov instability (Richtmyer 1960; Meshkov 1969; Brouillette & Sturtevant 1993). As the shock is stalled, material near its front converts from nucleons to helium. Nucleons are more accelerated by a given pressure gradient than He nuclei; the gradient in the concentration of nucleons is precisely the condition for Richtmyer-Meshkov, and the sign of the gradient does not matter. This strong instability will grow rapidly. Once the dying shock is in convection, this will infect the infalling material.

The Richtmyer-Meshkov instability is helpful, but it is not necessary: Herant et al. obtain convection from the Schwarzschild instability,  $dS/dr < 0$ , alone. So there are ample reasons to start convection in the dying shock where it can start fairly early. Rapid start of convection is decisive, e.g., to distinguish Herant convection from that of Miller et al. (1993) (see § 1). Therefore, the problem of the start of convection should be further and carefully investigated, probably by a two-dimensional computation including all relevant physical parameters. Also the "infection" of the new, infalling material by the convecting, dying shock must be investigated further.

The negative entropy gradient,  $dS/dr < 0$ , arises directly from the fact that the prompt shock is dying. As it progresses, the shock front loses pressure and temperature. Since this causes convection, which, together with neutrino heating, revives the shock, we may say that the death of the prompt shock causes its own rebirth. The short timescale of the rebirth,  $\sim 0.1$  s, helps this process.

The negative  $dS/dr$  is enhanced by the fact that the material at larger  $r$  is He, while that at smaller  $r$  is nucleons. The effect of this is discussed in Appendix B.

There is ample negative  $dS_{\text{eff}}/dr$  in the dying prompt shock. Infalling cold material encounters the convecting prompt shock and will participate in the convection.

### 16. $Y_e$ IN THE NUCLEOSYNTHESIS REGION

The product of nucleosynthesis is very sensitive to  $Y_e$  (S. E. Woosley 1992, private communication). In order to get  $^{56}\text{Ni}$  rather than some more neutron-rich nucleus like  $^{54}\text{Fe}$ , we need  $Y_e > 0.495$ . How can this be achieved?

We shall first assume that the ejecta undergoing nucleosynthesis all originated from infalling material, not from material which was originally in the proto-neutron star. The infalling material which undergoes nucleosynthesis and is then ejected is probably half oxygen and half silicon. This is the result of the presupernova calculation of Woosley. I assume the same isotopic composition as in atmospheric O<sub>2</sub>, i.e., 0.04%  $^{17}\text{O}$  and 0.20%  $^{18}\text{O}$ ; this means

$$Y_e = 0.50 - 1.4 \times 10^{-4}. \quad (16.1a)$$

The deviation from  $\frac{1}{2}$  is essentially negligible. For Si, which according to presupernova calculations by Nomoto is the re-

vant infalling material, again assuming the same isotopic composition as on Earth, the initial value is

$$Y_e = 0.50 - 2 \times 10^{-3}, \quad (16.1b)$$

not quite as "safe" for  $^{56}\text{Ni}$  production as equation (16.1a).

This  $^{16}\text{O}$  and/or Si is then irradiated by neutrinos. I assume, as before, a neutrino luminosity in  $v_e + \bar{v}_e$  of

$$L = 28 \text{ foe s}^{-1}. \quad (16.2)$$

The number of neutrinos at a distance  $R$  from the center is

$$\begin{aligned} F &= \frac{L}{4\pi R^2 \epsilon} = \frac{56 \times 10^{51}}{4\pi \times 10^{16} \times 1.6 \times 10^{-6} R_8^2 \epsilon} \\ &= \frac{2.8 \times 10^{41}}{R_8^2 \epsilon} \text{ cm}^{-2} \text{ s}^{-1}, \end{aligned} \quad (16.3)$$

where  $\epsilon$  is the average neutrino energy in MeV. The cross section for neutrino capture by a nucleon is

$$\sigma = 0.9 \times 10^{-43} \epsilon^2. \quad (16.4)$$

Thus the rate of neutrino capture by a nucleon (taking into account that a proton can only capture  $\bar{v}_e$ ) is

$$\lambda_n = \frac{0.013\epsilon}{R_8^2} \text{ s}^{-1}. \quad (16.5)$$

Setting  $\epsilon = 16$ , the measured value, we have

$$\lambda_n = \frac{0.20}{R_8^2} \text{ s}^{-1}. \quad (16.6)$$

If the gas consisted of nucleons, this would be the rate at which a nucleon would change from neutron to proton or vice versa.

The luminosity is not quite equal in  $v_e$  and  $\bar{v}_e$ , but, according to the computations by Wilson & Mayle (1989),  $\bar{v}_e$  is about 10% greater than  $v_e$ ; thus

$$L(\bar{v}_e) - L(v_e) \approx 0.05[L(\bar{v}_e) + L(v_e)]. \quad (16.7)$$

Therefore, the rate of change of  $Y_e$  would be, if we had free nucleons,

$$-\frac{dY_e}{dt} = \frac{0.010}{R_8^2}. \quad (16.8)$$

In complex nuclei in the neighborhood of Ni, the matrix element for capture is smaller; I estimate that this reduces the rate by about a factor of 10. Using also

$$v \approx 10^9 \text{ cm s}^{-1}, \quad (16.9)$$

and integrating from an initial  $R$  outward, we find

$$-\delta Y_e = \frac{10^{-3}}{R_8 v_8} = \frac{10^{-4}}{R_8}. \quad (16.10)$$

Even for the initial position  $R_8 = 0.3$ , this is negligible. So material originating outside will retain  $Y_e$  very close to 0.50.

The situation is totally different for material coming from inside, from the dying shock. This starts out from  $Y_e = 0.1-0.3$  and will stay at this level while moving out. Thus, if any of this material reaches the region of nucleosynthesis, the maximum amount permissible is given by

$$M_{\text{int}} < \frac{0.005}{0.3} \approx 2\%. \quad (16.11)$$

At most 2% of the material in the synthesis region is allowed to come from the dying shock. Taking the mass in the synthesis region to be given by the  $^{56}\text{Ni}$  formed,  $1.5 \times 10^{32}$  g, we find that the mass of interior material permitted to reach the synthesis region is limited to

$$M_{\text{int}} < 3 \times 10^{30} \text{ g}. \quad (16.12)$$

The mass in the dying shock beyond 100 km may be obtained from the calculations by Herant et al. and is

$$M_{\text{shock}} = 2.4 \times 10^{32} \text{ g}. \quad (16.13)$$

Thus only about 1% of this mass is permitted to get into the synthesis region; the rest must return to the neutron star.

Thus, we get a strong constraint on the convection: we need the dying shock to seed the convection (§ 15). But then the convection must bring only a very small fraction of the dying shock material into the synthesis region, i.e., the region from about 1000 to 5000 km.

## 17. CONCLUSIONS

1. Most important, the vigorous convection of Herant et al. gives a successful supernova shock. The structure of this shock, derived from the computation, is confirmed by the analytic treatment, energy is accumulated in the convective material until the Hugoniot equation can be fulfilled (§ 6). The subsequent supply of energy to the shock is small (§ 7).

2. The main reason why the convection model succeeds is that it permits the energy derived from neutrino heating to accumulate in the region behind the shock. The one-dimensional treatment makes the heated material accrete to the neutron star, where it is useless. The theory with convection also permits fresh infalling material to penetrate into the convecting region while the shock energy is being built up, and even when the shock is moving out.

3. The most important contribution to the shock energy is proportional to the rate of mass flow to the center (see eq. [6.12]). This rate in turn is likely to be proportional to the value of  $H = pr^3$  in the presupernova star in the region which will come to the center at the time the shock is formed. This part of the shock energy is essentially independent of the neutrino luminosity  $L$ , provided that this exceeds a certain minimum value. A smaller contribution depends on the neutrino luminosity.

4. An appreciable amount of energy, about 0.2 foe, is contributed by nucleosynthesis, some by synthesis of  $^{56}\text{Ni}$  and some by synthesis of Si and S.

5. It is very important that some energy is temporarily stored in dissociation of nuclei and subsequently recovered (§ 12).

6. The fact that the main contribution to energy is proportional to the infalling density,  $\rho_1 r^3$ , should be useful for calculating supernovae in stars of different mass.

I am very grateful to Marc Herant, Willy Benz, and Stirling Colgate for sending me this paper before publication and for several very useful discussions. I would also like to thank J. Wilson and R. Mayle for repeatedly sending me their computer outputs and for discussions. My thanks are due to Stan Woosley, who has patiently instructed me on the basic features of supernovae. Finally, I wish to thank the Institute for Theoretical Physics at Santa Barbara, where some of this work was done, for their hospitality.

APPENDIX A  
CALCULATION OF  $\eta$

In order to estimate  $\eta$ , I assume that the shock, and surfaces of constant pressure are approximately spherical. Then, on one such surface, the density  $\rho$  is given by the temperature, because

$$P/\rho \sim T/\mu, \quad (A1)$$

where  $\mu$  is the average molecular weight,

$$\frac{1}{\mu} = \sum_i \frac{X_i}{A_i}, \quad (A2)$$

where  $X_i$  is the mass fraction in particles of type  $i$ , and  $A_i$  is their effective atomic weight. As always in astrophysics, in calculating  $A_i$ , enough electrons must be included to make the matter neutral. Thus  $A_i = 1/2$  for protons,  $A_i = 4/3$  for  $\alpha$ -particles, but  $A_i = 1$  for neutrons. A mixture of equal numbers of neutrons and protons has

$$\frac{1}{\mu_u} = \frac{1}{2} (1 + 2) = \frac{3}{2}. \quad (A3)$$

A mixture of equal mass fractions of such nucleons and  $\alpha$ -particles has

$$\frac{1}{\mu_d} = \frac{1}{2} \left( \frac{3}{2} + \frac{3}{4} \right) = \frac{9}{8}. \quad (A4)$$

The upstream is likely to have a temperature such that energy gain by neutrino capture equals energy loss by electron capture. According to Paper I (eq. [7.2]), this means

$$T^3 r_7 \approx 7. \quad (A5)$$

Since  $r_7$  is somewhat greater than unity,

$$T \leq 2, \quad (A6)$$

so, using equation (A3),

$$(T/\mu)_u \leq 3. \quad (A7)$$

The downstream, having, by assumption,  $X_n = X_\alpha = 1/2$ , has a temperature of about 1 MeV; then, using equation (A4),

$$(T/\mu)_d = \frac{9}{8}. \quad (A8)$$

Hence the ratio of densities, according to equation (A1), is

$$\rho_d/\rho_u = 3 \times 8/9 = 8/3. \quad (A9)$$

The volume occupied by the downstream is thus 3/8 times that occupied by the upstream, or 3/11 of the total. The ratio of solid angles occupied by the two streams would be the same if the streams were exactly vertical (radial).

In the two-dimensional computation, and presumably in reality, this is not the case, but the motion is more random. This favors exposure of the downstream, justifying the assumption

$$\eta \approx \frac{1}{3}. \quad (A10)$$

In § 12 we pointed out that not all the infalling material is turned around into the upstream, but only a fraction  $\lambda$  (perhaps 50 %), while the fraction  $1 - \lambda$  accretes to the neutron star. Hence 1 gram of matter will occupy a volume  $1/\rho_d$  in the downstream, but only  $\lambda$  grams will go into the upstream, where they will occupy a volume  $\lambda/\rho_u$ . Thus the ratio of volumes occupied, and of solid angle subtended in case of vertical streams, is

$$\frac{\rho_u}{\lambda \rho_d} = \frac{3}{8\lambda}. \quad (A11)$$

The fraction of the total solid angle subtended by the downstream is then

$$f = \frac{3}{8\lambda + 3}. \quad (A12)$$

This is then the fraction of the total possible neutrino energy which the downstream receives. But only a fraction  $\lambda$  of this goes to the upstream, so

$$\eta_{\text{eff}} = f\lambda = \frac{3\lambda}{8\lambda + 3}. \quad (A13)$$

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For  $\lambda = \frac{1}{2}$ , as surmised in § 12, this is

$$\eta_{\text{eff}} = \frac{3}{14} = 0.21 , \quad (\text{A14})$$

compare with 3/11 for  $\lambda = 1$ . Considering that the streams are not vertical, the estimate  $\eta = 1/3$  is still reasonable.

## APPENDIX B

## ENTROPY AT THE H-He INTERFACE

According to statistical mechanics, the entropy in a hot and dense gas is roughly the same per particle, regardless of the weight of the particle. At  $T \approx 1$  MeV and  $\rho \approx 10^8$ , this entropy per particle is about  $12k_B$ , rather insensitive to  $T$  and  $\rho$ . Thus, if the material is nucleons, the entropy is  $12k_B \text{ nucleon}^{-1}$ ; if it is  $\alpha$ -particles, it is  $3k_B \text{ nucleon}^{-1}$ . Thus, we automatically have a negative gradient of the nuclear entropy, from  $S_m = 12$  to  $S_m = 3$ , quite independent of a gradient due to heat content. However, convection does not simply depend on the total  $S = S_r + S_m$ .

To see this, let us assume that the radiation entropy  $S_r$  is constant, i.e., independent of  $r$ . The ratio of material pressure to radiation pressure can be derived by combining equations (5.5), (5.8), (5.9), and (5.12) of Paper I, and is

$$\frac{P_m}{P_r} = \frac{4}{S_r} \quad (\text{B1})$$

if and only if the material is in the form of nucleons. If only a fraction  $X$  is nucleons and the rest  $\alpha$ -particles, the material pressure (at given  $\rho$  and  $T$ ) is multiplied by

$$X + \frac{1}{4}(1 - X) = \frac{1}{4}(1 + 3X) , \quad (\text{B2})$$

so

$$\frac{P_m}{P_r} = \frac{1 + 3X}{S_r} . \quad (\text{B3})$$

At a given level  $r$  in the star, the total pressure  $P$  is independent of  $X$ .

Let us now move a blob of material from low pressure  $P_1$  to higher pressure  $P_2$ , i.e., inward. The blob is assumed to keep its nucleon fraction  $X_1$ , but the ambient nucleon fraction  $X_2$  will be higher than  $X_1$ . The total pressure in the blob is

$$P = (P_r/S_r)(S_r + 1 + 3x) . \quad (\text{B4})$$

$$S_r = AT^3/\rho , \quad (\text{B5})$$

with  $A$  a numerical factor, while

$$P_r = BT^4 , \quad (\text{B6})$$

$$P_r/S_r = BA^{-1}T\rho . \quad (\text{B7})$$

We have assumed that  $S_r$  is constant, and so is the same in the "blob" and in the outside material. With  $S_r$  given,

$$T \sim \rho^{1/3} , \quad (\text{B8})$$

$$\rho T = C\rho^{4/3} , \quad (\text{B9})$$

with  $C$  the same in both materials. Hence equality of pressure in both materials means

$$\rho_1^{4/3}(S_r + 1 + 3X_1) = \rho_2^{4/3}(S_r + 1 + 3X_2) . \quad (\text{B10})$$

Since  $X_2 > X_1$ , it follows that  $\rho_1 > \rho_2$ . The blob which has been moved down has a higher density than the ambient, thus it will fall farther, and we get convection.

Quantitatively, setting  $X_1 - X_2 = \delta X$ ,  $\rho_1 - \rho_2 = \delta\rho$ , and considering these quantities small, we get

$$\frac{4}{3} \frac{\delta\rho}{\rho} = - \frac{3\delta X}{S_r + 1 + 3X} . \quad (\text{B11})$$

This gives the buoyancy of material with higher nucleon content. We expect convection to take place between the nucleon region at about 150 km and the region  $X = \frac{1}{2}$ . Assuming  $S_r = 5$ , corresponding  $\delta\rho/\rho$  is 20%, so we get vigorous convection.

To prevent convection, it would be necessary to have  $\rho_1 = \rho_2$ . According to equation (B10), this requires

$$S_r + 3X = \text{constant} . \quad (\text{B12})$$

Now the material (nuclear) entropy (per nucleon) changes from about 3 to 12 as  $\alpha$ -particles turn into nucleons: thus

$$S_m = 3 + 9X , \quad (\text{B13})$$

hence equation (B12) may be rewritten

$$S_{\text{eff}} = S_r + S_m/3 = \text{constant} . \quad (\text{B14})$$

The proper Ledoux criterion thus involves  $S_r + S_m/3$ , not  $S_r$  itself or the total entropy. In equilibrium, equation (B14) holds. A similar relation is true in going from He to still heavier nuclei.

## APPENDIX C LOCATION OF NUCLEOSYNTHESIS

The location of nucleosynthesis may be calculated. To form  $^{56}\text{Ni}$ , we need a temperature of at least  $350 \text{ keV} = 4.0 \times 10^9 \text{ K}$ . If the shock front has this temperature (and  $Y_e$  is sufficiently close to 0.50),  $^{56}\text{Ni}$  will be formed. Afterward, as the material cools down,  $^{56}\text{Ni}$  will be preserved because it is the most stable nucleus with equal numbers of neutrons and protons.

The radiation pressure at 350 keV is

$$P_r = 1.26 \times 10^{26} T^4 = 1.9 \times 10^{24} \text{ ergs cm}^{-3} \quad (\text{C1})$$

(pressure from electron pairs is included here). I neglect the material pressure for nuclear material. The energy in the shock is related to  $P$  by the virial theorem (eq. [6.2]).

$$4\pi P_s R_s^3 = E_s + A . \quad (\text{C2})$$

We take  $E_s = 1.4 \text{ foe} = 14 \times 10^{50} \text{ ergs}$ , and  $P_s$  from equation (C1); then

$$R_s^3 = 7.4 \times 10^{25} \text{ cm}^3 , \quad R_s = 4200 \text{ km} . \quad (\text{C3})$$

Herant et al. followed the shock out to 3000 km. Therefore, they did not include the synthesis of Si and S. They may have included the energy from synthesis of Ni. Their energy should be increased by 0.1–0.2 foe, to 1.5 foe for the  $15 M_\odot$  star.

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**Breakout of the Supernova Shock**  
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Several 2D computations of the Supernova Shock had been published, with contradictory results. This paper shows that the breakout occurs due to recombination of nucleons into  $\alpha$ -particles, and that this recombination indeed occurs at about 300 km. After breakout, the shock moves with a velocity of the order of  $10^4 \text{ km s}^{-1}$ .

## BREAKOUT OF THE SUPERNOVA SHOCK

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### ABSTRACT

The shock in a supernova of Type II first moves slowly and then suddenly breaks out with a velocity of order  $10^9 \text{ cm s}^{-1}$ . This breakout is due to the recombination of nucleons into  $\alpha$ -particles. It is shown that this recombination provides enough energy to lift the matter against gravity. The net energy after escape from the star is about  $4 \times 10^{18} \text{ ergs g}^{-1}$ . Supernovae of Type II differ mainly in the binding energy of the mantle of the progenitor.

*Subject headings:* nuclear reactions, nucleosynthesis, abundances — shock waves — supernovae: general

### 1. INTRODUCTION

The basic source of supernova energy is neutrinos from the core. Some of these are absorbed by matter in the region between about 100 and 300 km and give their energy to this matter. The material gets to this region by accretion; in fact, from a certain time on, most of the accreting material stays in this region.

There are two additional requirements for a successful supernova shock, namely (1) vigorous convection in the region from 100 to 300 km and (2) rather high density in that region. The convection has been treated by two-dimensional computations (Herant et al. 1994; Burrows, Hayes, & Fryxell 1995; Janka & Müller 1995). Wilson, Miller, & Mayle (1995) have treated the convecting region in a one-dimensional computation, using a mixing length scheme. This treatment, while potentially not as accurate as a two-dimensional computation, is particularly valuable for our purpose because it gives density, temperature, and entropy as a function of just two variables, radius  $r$  and time  $t$ .

Concerning density, I have shown (Bethe 1995, hereafter Paper II) that, in order to achieve a supernova energy of about  $10^{51} \text{ ergs}$ , the amount of matter in the convecting region must be about  $4 \times 10^{32} \text{ g}$ . This requires

$$\rho r^3 > 10^{31}. \quad (1.1)$$

Since the density is high, the entropy in radiation, which is proportional to  $T^3/\rho$ , cannot be very high.

Accretion builds up the material in the convection region slowly and thus drives the accretion shock out slowly. Typical velocities, from numerical computations, are of order  $2000 \text{ km s}^{-1}$ . Again, using numerical computations, at some time the shock suddenly accelerates to a velocity of the order of  $10,000 \text{ km s}^{-1}$ , when it breaks out and becomes a true outgoing shock.

This paper discusses the mechanism of this breakout. The breakout comes about by the recombination of nucleons into  $\alpha$ -particles; the energy thus released is converted into gravitational potential energy. As was shown in Paper II, this can only happen when the gravitational potential is less than the binding energy of  ${}^4\text{He}$ , which means at  $R \approx 300 \text{ km}$ .

The dissociation of  $\alpha$ -particles is, of course, not a primary source of energy; the neutrinos from the core are that primary source. However, the dissociation into nucleons serves as a temporary storage of the energy, to make it readily available for driving the shock.

### 2. SAHA

We consider a piece of material at  $R_1 = 300 \text{ km}$  in which a fraction  $X_1 = 0.75$  is dissociated into nucleons, while  $1 - X_1 = 25\%$  is  $\alpha$ -particles. We move it up, against gravity, such that the fraction of nucleons is decreased to  $X_2 = 0.25$ . These fractions are chosen because  $X$  changes fastest with temperature in this range.

The fraction of dissociation is given by the Saha equation:

$$\frac{n_p^2 n_n^2}{n_\alpha} = \left( \frac{m_p k T}{2\pi\hbar^2} \right)^{9/2} \left( \frac{m_n}{m_\alpha} \right)^{3/2} 2^4 \exp - \frac{Q}{kT}, \quad (2.1)$$

where  $n_p$ ,  $n_n$ , and  $n_\alpha$  are the numbers per  $\text{cm}^3$  of protons, neutrons, and  $\alpha$ -particles,  $m_p$ ,  $m_n$ , and  $m_\alpha$  are their respective masses, and  $Q = 28.3 \text{ MeV}$  is the dissociation energy of the  $\alpha$ -particle;  $2^4$  is the statistical weight of the nucleons due to spin. For simplicity, we assume  $n_p = n_n$ ; we then have

$$\begin{aligned} n_p &= 6 \times 10^{23} \rho X / 2, \quad n_\alpha = (6 \times 10^{23}/4)\rho(1-X), \\ (3 \times 10^{23})^3 \rho^3 \frac{X^4}{1-X} &= (3.80 \times 10^{23} T)^{9/2} \exp \left( -\frac{28.3}{T} \right), \end{aligned} \quad (2.2)$$

where  $T$  is in MeV.

If we assume  $T_1 = 1.20 \text{ MeV}$  at  $R_1$  and  $X = 0.75$ , then

$$\rho \equiv \rho_1 = 3.6 \times 10^8 \text{ g cm}^{-3}, \quad (2.3)$$

which is about the correct density inside the shock; see Paper II. ( $T$  is very insensitive to  $\rho$ .) Moving from  $X = 0.75$  to 0.25, the major part of the pressure is due to radiation (see § 3), so  $\gamma \approx 4/3$ ; this is also a fair approximation to the material pressure because of the transformation of  $\alpha$ -particles into nucleons with increasing temperature. Therefore, we take

$$\rho T^{-3} = \text{const.} \quad (2.4)$$

This is well confirmed by numerical computations (Wilson et al. 1995). Our numbers above, viz.,  $T = 1.20$  and equation (2.3), give

$$\rho T^{-3} = 2.08 \times 10^8. \quad (2.5)$$

With this assumption and  $X = 0.25$ , the Saha equation (2.2) gives

$$T = T_2 = 0.94 \text{ MeV}, \quad (2.6)$$

$$\rho_2 = 0.26 \times 10^8. \quad (2.7)$$

The transformation from 75% nucleons to 75%  $\alpha$ -particles thus extends over a temperature interval

$$\Delta T = T_1 - T_2 = 0.26 \text{ MeV}. \quad (2.8)$$

### 3. MECHANICAL EQUILIBRIUM

We assume hydrostatic equilibrium,

$$-\frac{\partial P}{\partial r} = \frac{GM}{r^2} \rho. \quad (3.1)$$

(The acceleration term is relatively small; see the end of this section.) We write equation (3.1) in the form

$$-\frac{dP}{\rho} = GM \frac{dr}{r^2}. \quad (3.2)$$

The pressure consists of the material pressure  $P_m$  and the radiation pressure  $P_r$ , which includes the pressure of the relativistic electrons and positrons. The material pressure therefore is due only to the heavy particles:

$$P_m = 0.96 \times 10^{18} T \rho [\frac{1}{4}(1-X) + X] \text{ ergs cm}^{-3}. \quad (3.3)$$

We take  $X$  equal to its average value in the interval considered,  $X = \frac{1}{2}$ ; then

$$P_m = 0.60 \times 10^{18} T \rho. \quad (3.4)$$

The pressure of radiation plus electrons was put into a convenient form in an earlier paper (Bethe 1993, hereafter Paper I); equations (5.6) and (5.8) of that paper state

$$P_r = (1.26 + 0.35\eta^2 + 0.017\eta^4) \times 10^{26} T^4 \text{ ergs cm}^{-3}, \quad (3.5)$$

where  $\eta$  is given by

$$\rho Y_p T^{-3} = 0.72 \times 10^8 \eta(1 + \eta^2 \pi^{-2}). \quad (3.6)$$

Here  $Y_p$  is the fraction of protons among all nucleons, bound and free; we set  $Y_p = 0.50$ . Comparing equations (2.5) and (3.6),

$$\eta = 1.05, \quad (3.7)$$

and inserting this value into equation (3.5), we obtain

$$\frac{P_r}{\rho} = 1.00 \times 10^{18} T. \quad (3.8)$$

Adding equation (3.4), we find

$$P/\rho = 1.60 \times 10^{18} T \equiv BT. \quad (3.9)$$

Inserting this into equation (3.2), we obtain

$$\frac{dP}{P} BT = GM d(r^{-1}). \quad (3.10)$$

We have previously, in equation (2.4), found that  $\gamma = 4/3$ ; hence,

$$dP/P = 4dT/T. \quad (3.11)$$

Then equation (3.10) can be integrated to give

$$4B\Delta T = \Delta(GMr^{-1}). \quad (3.12)$$

The right-hand side is the difference of gravitational potential between levels 1 and 2. The left-hand side, using equations (3.9) and (2.8), is

$$4B\Delta T = 6.4 \times 10^{18} \Delta T = 1.67 \times 10^{18} \text{ ergs g}^{-1}. \quad (3.13)$$

This then is the energy required to lift the matter from level 1 to level 2.

To accomplish this, we have available:

1. One-half the  $\alpha$ -particle dissociation energy, i.e., 3.5 MeV per nucleon.

2. The difference in thermal energy in heavy particles, 0.85 MeV per nucleon. This is mainly due to the reduction in number of particles, due to recombination. Together, these give

$$4.4 \text{ MeV nucleon}^{-1} = 4.2 \times 10^{18} \text{ ergs g}^{-1}. \quad (3.14)$$

3. The difference in thermal energy in radiation,

$$\Delta\epsilon_r = 3\Delta(p/\rho) = 3(1.0 \times 10^{18})0.26 = 0.79 \times 10^{18} \text{ ergs g}^{-1}$$

$$\text{Total } \Delta\epsilon = 5.0 \times 10^{18} \text{ ergs g}^{-1}. \quad (3.15)$$

This is much more than the required gravitational energy, given by equation (3.13). The difference is ample to provide the kinetic energy for a mean velocity of  $10^9 \text{ cm s}^{-1}$ ,

$$\epsilon_{\text{kin}} = 0.5 \times 10^{18} \text{ ergs g}^{-1}, \quad (3.16)$$

plus potential energy to lift the (small amount of) matter which originally is located between 300 and 430 km (about  $0.01 M_\odot$ ). However, it is also clear that the necessary gravitational energy could not be provided without the recombination of  $\alpha$ -particles.

We conclude: once the shock gets into the region where nucleons combine into  $\alpha$ -particles, the energy set free by this recombination is amply sufficient to lift the matter out of the gravitational hole. It is this recombination which makes the shock break out, not an instability in the stellar dynamics (Burrows & Goshy 1993), nor a decline of ram pressure.

In order to begin rapid recombination into  $\alpha$ -particles, we need a temperature  $T \leq 1.2 \text{ MeV}$ . Our result shows that  $R = 300 \text{ km}$  is satisfactory, as surmised in Paper II.

From equation (3.10), we can calculate the radius at level 2, i.e., where the fraction of nucleons has decreased to 0.25. The baryonic mass enclosed by our region of recombination is about  $1.5 M_\odot$ , according to the computations. In equation (3.10),  $M$  is the gravitational mass, about  $1.35 M_\odot$ , so  $GM = 1.8 \times 10^{26}$ . The left-hand side of equation (3.10) is given by equation (3.13), so

$$\Delta(r^{-1}) = 10^{-8} \text{ cm}^{-1}. \quad (3.17)$$

Thus, if the inner radius is  $3 \times 10^7 \text{ cm}$ , the outer radius is given by

$$r_2^{-1} = (3.3 - 1.0) \times 10^{-8} \text{ cm}^{-1}, \\ r_2 = 430 \text{ km}. \quad (3.18)$$

This result is sensitive to the detailed assumptions, viz.,  $R_1 = 300 \text{ km}$  and  $T_1 = 1.2 \text{ MeV}$ , but nothing in the following sections will depend on  $r_2$ .

### 4. ENERGY

In § 3 we have shown that the recombination of nucleons into  $\alpha$ -particles gives sufficient energy to lift the material out of the gravitational potential hole. However, § 3 should not be used to calculate the energy of the supernova. To do this, we must consider the energy balance in going from 300 km to infinity.

The components of energy are the following:

75% of the full dissociation energy of $\alpha$ -particles	5.3 MeV nucleon $^{-1}$ ;
Recombination energy <sup>1</sup> of $\alpha$ 's into $^{16}\text{O}$	0.9 MeV nucleon $^{-1}$ ;
Thermal energy of baryons for $X = \frac{3}{4}$ , $T = 1.2$	1.5 MeV nucleon $^{-1}$ ;
Thermal energy in radiation	2.2 MeV nucleon $^{-1}$ ;
minus gravitational potential energy at 300 km	6.2 MeV nucleon $^{-1}$ ; 3.7 MeV nucleon $^{-1}$ ;
	$\epsilon = 3.5 \times 10^{18} \text{ ergs g}^{-1}$ . <span style="float: right;">(4.1)</span>

Thus, to get a total energy of 1 foe =  $10^{51}$  ergs, we need a total mass in the shock of

$$M_{\min} = 2.8 \times 10^{32} \text{ g} = 0.14 M_{\odot}. \quad (4.2)$$

Some energy is added to the shock by nucleosynthesis and by neutrino absorption after breakout. In Paper II this has been estimated as 0.4 foe.

However, then the shock has to overcome the binding energy of the mantle of the progenitor—let us say, the matter beyond  $M_r = 2 M_{\odot}$ . For heavy stars, this has been estimated by Woosley & Weaver (1995) and can be approximated by

$$-E_{\text{env}} = 0.06(MM_{\odot}^{-1} - 5) \text{ foe}, \quad (4.3)$$

provided  $M/M_{\odot} > 20$ . If  $M/M_{\odot} > 30$ , this binding energy is greater than 1.5 foe. Provided the initial energy of the shock is 1 foe or less, it is completely used up in trying to expel the envelope; in other words, the shock gets stuck. The star will then presumably collapse into a black hole, in agreement with the conclusion by Woosley & Weaver. However, the energy of the shock at breakout should still be investigated as a function of the progenitor mass.

##### 5. NEED FOR $\alpha$ RECOMBINATION

Breakout cannot be achieved by thermal energy, whether in relativistic or in heavy particles. The latter is simply pro-

<sup>1</sup> I have assumed in my previous paper that  $^{16}\text{O}$  is the initial state of the matter before collapse and is the standard from which nucleosynthesis energies are calculated.

portional to  $T$ . Radiation and relativistic particles have an energy (per unit mass) of  $T^4/\rho$ . But in the presence of electrons, as has been shown in Paper II (§ 5)

$$\rho \sim T^3, \quad (5.1)$$

so that the relativistic particle energy is also proportional to  $T$ . The only condition is that  $Y_p$  be constant, where  $Y_p$  is the ratio of the total number of protons (bound and free) to the total number of nucleons (bound and free).

Paper I further shows that for constant entropy,

$$T = K/r_7 + b. \quad (5.2)$$

If the chemical composition remains constant, i.e., if there is no recombination of nucleons into  $\alpha$ -particles, this relation holds for all  $r$ . For large  $r$ ,  $T$  must go to 0, then  $b = 0$ . Thus, for no change of composition, the thermal energy per unit mass is

$$\epsilon_{\text{th}} \sim 1/r. \quad (5.3)$$

The gravitational potential energy is likewise proportional to  $1/r$ . Therefore, if the sum of gravitational and thermal energy is negative in the convection region, as it is in fact, it will remain negative for all  $r$ , and the shock cannot break out.

The dissociation energy, by contrast, is independent of  $r$ , and thus will win at sufficiently large  $r$ .

##### 6. CONCLUSION

The dissociation energy not only causes the breakout of the shock, but also provides the bulk of the starting energy of the shock (§ 4). Of course, as pointed out in § 1, the dissociation is not the basic source of energy, but is only the temporary storage of energy.

If this is so, the initial energy per unit mass in the shock should be essentially the same for all Supernova of Type II. The initial shock energy is then proportional to the mass which can be assembled between the entropy maximum and the shock. This mass may depend on the details of the presupernova density distribution, but its computation is less time-consuming than a full supernova computation.

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## **List of Publications**

1. Theorie der Beugung von Elektronen an Kristallen (Theory of the Diffraction of Electrons by Crystals), *Ann. Physik* **87**, 55–129 (1928)
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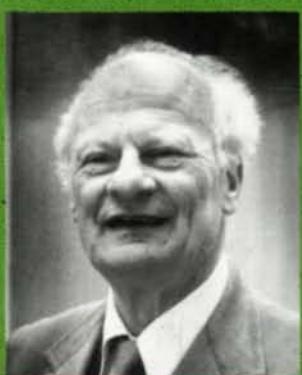
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Hans A Bethe received the Nobel Prize for Physics in 1967 for his work on the production of energy in stars. A living legend among the physics community, he helped to shape classical physics into quantum physics and increased the understanding of the atomic processes responsible for the properties of matter and of the forces governing the structures of atomic nuclei.

This collection of papers by Prof Bethe dates from 1928, when he received his PhD, to now. It covers several areas and reflects the many contributions in research and discovery made by one of the most important and eminent physicists of all time. Special commentaries have been written by Prof Bethe to complement the selected papers.

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