

LECTURES IN THEORETICAL PHYSICS
VOLUME I

THE LECTURERS

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LECTURES IN THEORETICAL PHYSICS

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INTRODUCTION

This volume contains lectures delivered at the first annual Summer Institute for Theoretical Physics held in the Department of Physics, University of Colorado, June 16 through August 22, 1958.

The Institute is sponsored jointly by the Air Force Office of Scientific Research (ARDC) and the University of Colorado with the cooperation of the Boulder Laboratories of the National Bureau of Standards. The inception of the Summer Institute is due mainly to the efforts of Prof. E. U. Condon, Washington University, St. Louis; Prof. A. B. Weaver, former physics department chairman at the University of Colorado who now heads the physics department at the University of Arizona, and to Prof. George Gamow of the University of Colorado.

The function of the Institute is to bring together scientists and students with the view of providing a means for exchange of ideas and information. Lectures, seminars and informal discussions make up the activities of the Institute.

The lecturers in some cases prepared the material herewith presented and in other cases edited and revised the notes which were taken during the lectures. Appreciation is expressed to the authors for their time-consuming work in the preparation of their manuscripts.

Credit for writing up notes is gladly given to A. Maschke, University of Nebraska; and John McCullen, Lee Schick and Arthur Sakakura, Department of Physics, University of Colorado. Thanks for doing well the difficult task of writing in equations is extended to Miss Jean Newman, Department of Physics, University of Colorado, Mr. Schick and Mr. McCullen. Special thanks is due Mr. McCullen for additional editorial assistance. Thanks for the painstaking job of typing is given to Mrs. Carolyn Ceriello.

Major Charles K. Reed, chief of the Nuclear Physics Division, U.S.A.F., deserves a great deal of credit for his helpful advice and suggestions which aided materially in making the Institute a success.

Editors,

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CONTENTS

INTRODUCTION	v
PAIR PRODUCTION AND BREMSSTRAHLUNG IN THE FIELD OF AN ATOM, F. Rohrlich	1
THEORY OF PARTICLES WITH ZERO REST-MASS, R. H. Good, Jr.	30
STRANGE PARTICLES AND THEIR INTERACTIONS, Berthold Stech	82
SOME ASPECTS OF THE STATISTICAL-MECHANICAL THEORY OF IRREVERSIBLE PROCESSES, Ryogo Kubo	120
MULTIPLE PRODUCTION OF MESONS AND A NONLOCAL THEORY OF FIELDS, G. Wataghin	204
SELECTED TOPICS IN NUCLEAR THEORY, R. E. Peierls	238
HIGH-ENERGY COLLISION THEORY, R. J. Glauber	315

PAIR PRODUCTION AND BREMSSTRAHLUNG IN THE FIELD OF AN ATOM*

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In a recent review¹ of the subject of pair production and bremsstrahlung in the field of free and bound electrons, the present state of our theoretical knowledge was discussed. It is the purpose of these lectures to present the salient features of this important field of applied quantum electrodynamics to graduate students who are in general not acquainted with field theory, but who want to be able to compare experimental data with various stages of approximation of our best available theoretical analysis. A number of details will therefore be given which are not found in the review article and some of the physical arguments will be studied further. Emphasis will be placed on the underlying physical model and on the accuracy of various approximate solutions of the problem. It will be pointed out how far theory has progressed to date and which problems are still awaiting a solution.

We study the processes of pair production and bremsstrahlung partly for their own sake, i. e., as interesting phenomena in themselves which must be compared with our theoretical knowledge of elementary processes, and partly because they are almost always present as part of the "background" when we study other processes. Only their thorough understanding will permit us to eliminate this background.

As we shall see, pair production and bremsstrahlung are closely related processes, despite their quite different appearance at first sight. For this reason we shall discuss them more or less in parallel.

In pair production, a photon collides with another particle and produces a negaton-positon pair while the struck particle recoils and the photon disappears. The struck particle may or may not be excited in the process. We shall here be concerned only with the case where the struck particle is an atom. However, in order to fully understand this rather complicated system, we shall have to discuss separately first the special cases where the struck particle is a nucleus and where it is a free electron.

With the notation (E, \vec{p}) for the energy and momentum of a particle we can represent pair production as shown in Fig. 1. Note that we use the units in which $\hbar = c = 1$.

In the process of bremsstrahlung an electron (usually a negaton)

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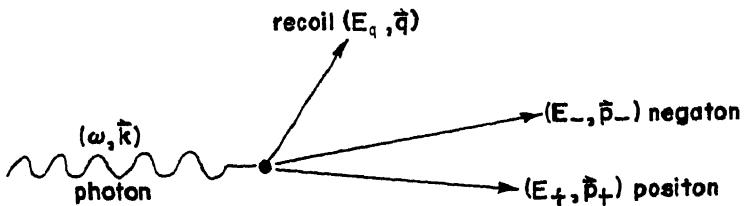


Fig. 1

collides with a charged particle (atom, nucleus, or electron) and, being scattered, emits a photon. The struck particle recoils, (cf. Fig. 2).

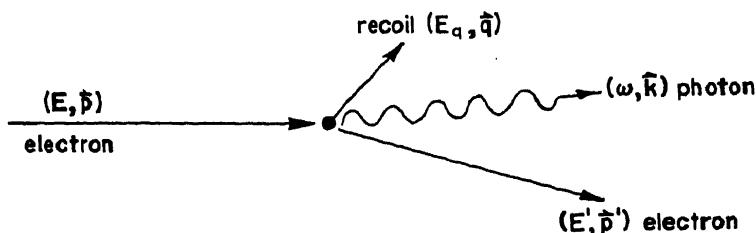


Fig. 2

The Bethe-Heitler Formulae

As a first approximation the atom is considered as stripped, consisting only of the nucleus. As we shall see, this is a good approximation, because the cross sections are proportional to the square of the charge of the struck particle. Since the nucleus yields $(Ze)^2$ which is in general much larger than the cumulative effect of the Z atomic electrons, Ze^2 , the error made in this approximation is of order $1/Z$. For very light atoms this approximation is poor and for Hydrogen one will expect to be in error roughly by a factor of 2. The cross sections for pair production and bremsstrahlung derived for a stripped infinitely heavy atom and in Born approximation are known as the Bethe-Heitler formulae.² They were first derived independently by Bethe and Heitler, Sauter, and Racah.

For pair production the conservation laws are

$$\omega = E_+ + E_-$$

$$\vec{k} = \vec{p}_+ + \vec{p}_- + \vec{q} \quad (1)$$

Energy conservation leads at once to a threshold energy $\omega_{\text{MIN}} = 2m$ below which pair production cannot take place: an obvious relationship. Momentum conservation shows that the recoil momentum is limited in magnitude from below as well as from above. Clearly,

$$\begin{aligned} q_{\text{MIN}} &= \omega - p_+ - p_- = (E_+ - p_+) + (E_- - p_-) \\ &\cong \frac{m^2}{2E_+} + \frac{m^2}{2E_-} = \frac{m^2 \omega}{2E_+ E_-} \equiv \delta \end{aligned} \quad (2)$$

The latter relation is valid for high energies ($\omega \gg 2m$). The upper recoil limit is $q_{\text{MAX}} \equiv 2\omega$ at high energies.

For bremsstrahlung the conservation laws

$$\begin{aligned} E &= E' + \omega \\ \vec{p} &= \vec{p}' + \vec{k} + \vec{q} \end{aligned} \quad (3)$$

show that the maximum radiated photon energy is $\omega_{\text{MAX}} = E - m$, and that its minimum is $\omega = 0$, in which case one has elastic scattering.

(Parenthetically, it must be pointed out that strictly speaking, the limit $\omega \rightarrow 0$ does not exist, since the finite energy resolution ΔE of an experiment will never permit one to exclude the possibility of emission of an undetermined number of very soft photons whose total energy does not exceed ΔE . Thus, elastic scattering of charged particles strictly speaking does not exist. The difficulties one encounters by ignoring this fact are known as the infrared divergence.)

The momentum conservation³ yields, as in pair production, a minimum recoil momentum

$$q_{\text{MIN}} \cong \frac{m^2 \omega}{2EE'} \equiv \delta \quad (4)$$

for high energies. It should be clear that the recoil momenta \vec{q} which we speak of here manifest themselves only as momentum transfers to the

nucleus, since the latter is assumed to be infinitely heavy and will not actually recoil.

As indicated by the threshold energy of about 1 Mev, pair production is a phenomenon which belongs in relativistic quantum electrodynamics. So does high energy bremsstrahlung. It is however possible, at least heuristically, to circumvent quantum field theory and derive the correct cross sections by means of standard quantum mechanical perturbation theory. This derivation we shall now sketch; it gives us a good physical picture and at the same time shows the close mathematical relationship between the two processes with which we are concerned.

The cross section $d\sigma$ is the ratio of the transition probability per unit time, $d\omega$, and the incident flux. The latter is equal to the velocity of the incident particle provided we normalize the density to one per unit volume. Thus, by a well-known formula of quantum mechanics

$$d\sigma = \frac{2\pi}{v} \overline{\sum} |M_{fi}|^2 d\Omega_f \quad (5)$$

where M_{fi} is the matrix element of the interaction in suitable order of perturbation theory, and $d\Omega_f$ is the density of final states per unit energy range. The symbol $\overline{\sum}$ indicates a summation over final states and an average over initial states. Normalizing in a volume $(2\pi)^3$,

$$\begin{aligned} d\Omega_f &= \frac{(2\pi)^3 p_+^2 dP_+ d\Omega_+}{h^3} + \frac{(2\pi)^3 p_-^2 dP_- d\Omega_-}{h^3} / dE_- \\ &= p_- E_- p_+ E_+ dE_+ d\Omega_+ d\Omega_- \end{aligned}$$

for pair production, and similarly,

$$d\Omega_f = p' E' \omega^2 d\omega d\Omega_k d\Omega'$$

for bremsstrahlung.

The Hamiltonian of the system is

$$H = H_o + H_i + H_{ext} \quad (6)$$

H_o = free electrons + free photons

$H_i = -\vec{J} \cdot \vec{A}$ = interaction of electrons with radiation field

$H_{ext} = \mp e \phi_{ext}$ = interaction of {positon} with nuclear static field

$$\Phi_{\text{ext}} = Z e/r.$$

Consider bremsstrahlung first. In a space-time diagram (time upwards) this process looks approximately as drawn in Fig. 3.

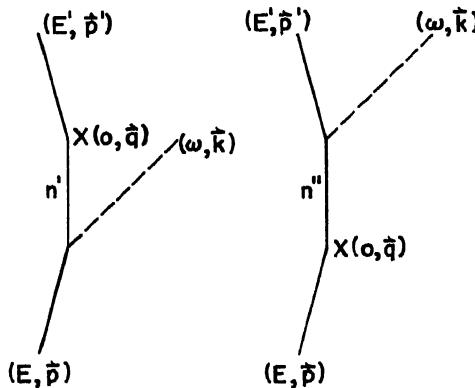


Fig. 3

Two possible intermediate states can occur, either the photon is first emitted and the electron is scattered afterwards, or the sequence is reversed. In either case, the intermediate state is a virtual state, since a photon cannot be emitted from a free particle without violating at least one conservation law. The photon emission takes place via the interaction H_1 , the scattering via H_{ext} . Thus, in second order perturbation theory (the lowest possible order for this process)

$$M_{fi} = \sum_{n'} \frac{(f|H_{\text{ext}}|n')\langle n'|H_1|i\rangle}{E_{n'} - E_i} + \sum_{n''} \frac{(f|H_1|n'')\langle n''|H_{\text{ext}}|i\rangle}{E_{n''} - E_i} \quad (7)$$

Momentum is conserved through the intermediate state (plane waves!), but the energies of the intermediate states are

$$E_{n'} = \omega + \sqrt{m^2 + (\vec{p} - \vec{k})^2}$$

$$E_{n''} = \sqrt{m^2 + (\vec{p}' + \vec{k})^2}.$$

Clearly, $E_t = E$. With M_{fi} thus determined it is a matter of straightforward algebra to carry out the spin and polarization sums in Σ and one obtains the Bethe-Heitler cross section for bremsstrahlung. Details of such a calculation can be found in Heitler's "Quantum Theory of Radiation."

Turning now to the corresponding calculation for pair production, we have the diagrams of Fig. 4.

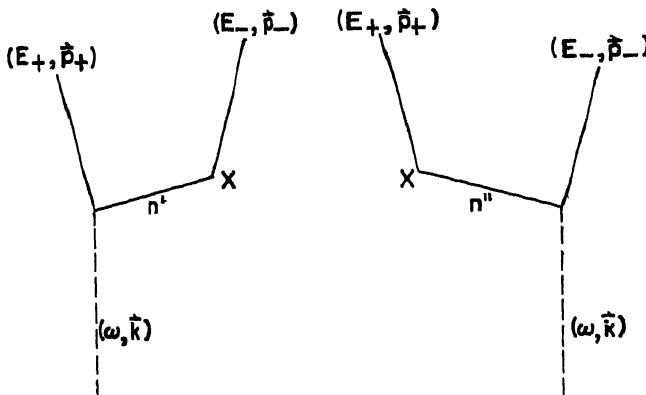


Fig. 4

The difference between the two possible processes here is that either the positon or the negaton may be scattered. Since a free photon cannot create a pair without violating at least one conservation law, the intermediate state must again be virtual. The expression for M_{fi} is formally identical with that for bremsstrahlung, the identification of states, however requires some thought.

The relativistic theory of electrons, based on the Dirac equation, tells us that the negaton and the positon can both be consistently described, provided one formally associates opposite charges with opposite signs of momentum and energy. Thus, if E_-, \vec{p}_- refer to a negaton, $E_+ = -E_-, \vec{p}_+ = -\vec{p}_-$ refer to a positon of the same energy. Since these signs infer a reversal of direction of motion, it follows that in scattering an outgoing negaton acts like an ingoing positon and v. v. Thus, this theory effectively tells us to replace Fig. 4 by the following Fig. 5 in which the outgoing positons are replaced by ingoing negatons of energy $-E_+$ and momentum $-\vec{p}_+$.

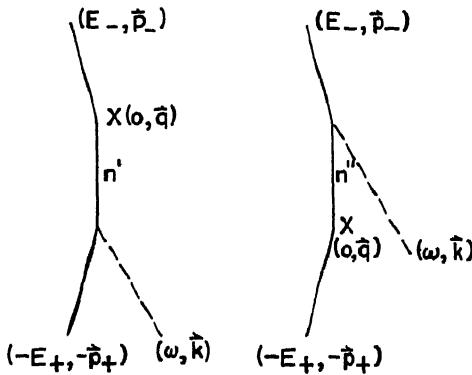


Fig. 5

A comparison of Fig. 5 with the diagrams for bremsstrahlung, Fig. 3, thus exhibits a relationship which can be summarized by the substitution:

bremsstrahlung	pair production
E', \vec{p}'	E_-, \vec{p}_-
E, \vec{p}	$-E_+, -\vec{p}_+$

(8)

M_{fi} for pair production now follows easily in the same way as for bremsstrahlung using Fig. 5. In particular,

$$E_{n'} = \sqrt{m^2 + (\vec{k} - \vec{p}_+)^2}$$

$$E_n = \omega + \sqrt{m^2 + (\vec{p}_- - \vec{k})^2}$$

$$E_i = -E_+ + \omega.$$

A comparison of the resulting M_{fi} for pair production with that for bremsstrahlung now exhibits an identity under the substitution (8) together with

$$\omega, \vec{k} \longrightarrow -\omega, -\vec{k} \quad (9)$$

which corresponds to the difference between Figs. 3 and 5 (outgoing photon replaced by ingoing photon).

The relationship between the M_{fi} of the two processes, expressed in (8) and (9), is a special case of the substitution law (cf. J. M. Jauch and F. Rohrlich, "Theory of Photons and Electrons").

I refer to Heitler's book for curves which show the various differential and total cross sections that emerge from the Bethe-Heitler formulae. For further reference, we shall quote here only two limits of the total cross section for pair production:

Near threshold ($\alpha = \text{fine structure constant}, r_0 = e^2/m$)

$$\sigma = \alpha r_0^2 Z^2 \frac{\pi}{12} \left(\frac{\omega}{m} - 2 \right)^3, \quad (10)$$

whereas in the high energy limit

$$\sigma = \alpha r_0^2 Z^2 \left(\frac{28}{9} \ln \frac{2\omega}{m} - \frac{218}{27} \right), \quad (11)$$

showing a logarithmic increase with energy.

Coulomb Corrections

The Bethe-Heitler formulae are computed in Born approximation. This means that initial, intermediate, and final states of the electrons are approximated by plane waves. In physical terms it means that we have made three simplifying assumptions. Since a Coulomb field makes itself felt even at arbitrarily large distances (by modifying plane waves into Coulomb waves), the incident and outgoing electrons are all the time under the influence of the nuclear Coulomb field. The Born approximation makes the apparently very strong assumption that this field acts only once for an instant.

The second assumption involved in this approximation is the neglect of the mutual interaction between the electrons, and the third one is the neglect of the interaction of each electron with itself. The second and third assumptions are actually related. They can be taken into account by computing higher order terms in the perturbation expansion. In quantum electrodynamics these terms are known as radiative corrections. These are of order α and are therefore well below present experimental accuracy and considerably smaller than various much more uncertain corrections to be discussed later.

We shall therefore restrict ourselves here to the discussion of the first of the three assumptions, i. e., the nuclear Coulomb field corrections.

For pair production this correction is very large near threshold. For example, numerical calculations for Pb at 1.3 Mev find the Born approximation to be too small by a factor of 2. No satisfactory methods have been devised so far to compute these corrections in the energy

region between threshold and about 10 or 20 Mev. The only method available is one of numerical computations which must be carried out separately for each energy and for each element. Even our best computing machines would have difficulties with this problem, because one is interested not only in the total cross section, but also in various differential cross sections containing quite a number of parameters such as angles and energies of the emerging particles.

For higher energies, beyond 20 Mev, say, the Born approximation for pair production is much better than might be anticipated. Experiments show a discrepancy of only 10 percent or less, depending on the energy and the element. This discrepancy can be satisfactorily removed by a method recently devised by Bethe, Davies, Maximon, and Olsen.³ They use approximate Coulomb wave functions which permit analytical treatment. The result is that the function

$$f(Z) = (\alpha Z)^2 \sum_{y=1}^{\infty} \frac{1}{y(y^2 + (\alpha Z)^2)} \quad (12)$$

has to be added to the logarithmic term in the cross section. We shall return to this point later (cf. Eqs. (26)). The correction adds to the Born approximation which is too low for high energies. (The Born approximation has accidentally the correct value--Coulomb correction is zero--at several Mev, depending on Z; e. g. for Pb. at 6 Mev). The remaining error due to Coulomb effects can be estimated to be of the order $(\alpha Z)^2 |\ln(\omega/m)/(\omega/m)|$.

Turning now to bremsstrahlung we find that the non-relativistic case is amenable to exact treatment including Coulomb effects, as was first shown by Sommerfeld. However, as one approaches the relativistic region one has similar difficulties as near the threshold of pair production. Approximate correction factors for the Born approximation exist (Elwert factor, Sommerfeld factor), but the problem is not solved. I understand that this question is now under study by Fano and co-workers and we can expect to have a much better understanding of the Coulomb correction in the near future.

At high energies, the methods of Bethe et. al. are again available and give again a relatively simple additive correction of the form (12).

Screening and the Coherent Scattering Function

So far we have only discussed the effect of the nucleus. The role which the atomic electrons play in the processes of pair production and bremsstrahlung is twofold and might be characterized crudely as static and dynamic effects.

The static effect of the atomic electrons is an effective shielding of the positive nuclear charge Ze, such that an incident or outgoing electron would see only a smaller effective charge $(Z-\sigma)e$. This effec-

tive charge will increase as the electron approaches the atom, because of the charge distribution of the atomic electrons. When the incident electron has penetrated the charge cloud of the atomic electrons and is well inside the first Bohr orbit it will see the whole nuclear charge. This effect of the atomic electrons is known as screening. It decreases the interaction and therefore the cross sections. Note that if only screening is taken into account the initial and final states of the atom are always the same. There is therefore no energy transfer to the atom, but only a momentum transfer. Under such conditions cross sections are said to be coherent.

However, the structure of an atom is such that any incident particle of sufficient energy can excite it or ionize it. If this happens, we speak of an energy transfer to the atom, and of an incoherent cross section. Both pair production and bremsstrahlung can be either coherent or incoherent.

In order to obtain a better understanding of screening it is useful to adopt a semiclassical picture of the collision process. The incident particle is assumed to have a more or less precise orbit. In particular, one assumes that--as in classical mechanics--one can associate to each incident particle an impact parameter b as well as a momentum p . By the uncertainty relation, $b = 1/q$, since q , the momentum transfer, is the change of the momentum p (roughly) perpendicular to its original direction. Clearly, this will be a good physical picture only for high energies.

The maximum impact parameter is given by the minimum momentum transfer (cf. Eqs. (2) and (4)), $b_{\text{MAX}} = 1/\sqrt{Z}$. Collisions with larger impact parameters cannot occur in pair production and bremsstrahlung and are thus irrelevant for the computation of the cross sections.

Now, let us describe our atom by the Thomas-Fermi model which will be satisfactory for all but the light elements. According to this model the neutral atom has a radius

$$a = a_0 / \sqrt{Z} \quad (13)$$

where $a_0 = 1/\alpha m$ is the Bohr radius. This radius is due to the screening of the nucleus by the atomic electrons. Without these electrons, this radius would be infinite. We can therefore characterize the effect of screening on the cross sections by a parameter which tells us whether or not the finiteness of a is relevant in the process. Clearly, when $b_{\text{MAX}} < a$, any size of $a > b_{\text{MAX}}$ will give the same cross section. But when $b_{\text{MAX}} > a$, then the finiteness of a will eliminate all impact parameters $a < b < b_{\text{MAX}}$. Thus,

$$\frac{a}{b_{\max}} = \alpha \delta = \begin{cases} \frac{m\omega}{2\alpha E_+ E_-} \cdot \frac{1}{Z^{1/3}} & \text{(pair production)} \\ \frac{m\omega}{2\alpha E E'} \cdot \frac{1}{Z^{1/3}} & \text{(bremsstrahlung)} \end{cases}$$

is a parameter characteristic of screening. It has become customary to replace $1/(2\alpha)$ by 100, and to define the screening parameter

$$\gamma = 200\alpha \alpha \delta = \begin{cases} \frac{100}{Z^{1/3}} \cdot \frac{m\omega}{E_+ E_-} & \text{(p. p.)} \\ \frac{100}{Z^{1/3}} \cdot \frac{m\omega}{E E'} & \text{(br.)} \end{cases} \quad (14)$$

The smaller γ , the larger is the screening effect. Thus, if the energies are low, screening is negligible. For $\gamma \gtrsim 10$ the screening correction will not exceed a few percent.

Classically, the potential energy due to the whole atom and an incident or outgoing electron at the position \vec{r} is

$$\pm V(\vec{r}) = - \frac{Ze^2}{r} + \sum_{i=1}^N \frac{e^2}{|\vec{r} - \vec{r}_i|} \quad \text{for a } \begin{cases} \text{negaton} \\ \text{positon} \end{cases} \quad (15)$$

where the summation is to be extended over all N atomic electrons ($N = Z$ for neutral atoms). The screened and unscreened cases differ exactly by the summation term.

Quantum mechanically, the nucleus is still regarded as a point source, but the electronic charge is distributed according to the ground state wave function of the atom, $\Psi_o(\vec{r}_1, \dots, \vec{r}_N)$. Thus,

$$\pm V_o(\vec{r}) = - \frac{Ze^2}{r} + \int \Psi_o^*(\vec{r}_1, \dots, \vec{r}_N) \sum_{i=1}^N \frac{e^2}{|\vec{r} - \vec{r}_i|} \Psi_o(\vec{r}_1, \dots, \vec{r}_N) d^3 r_1 \dots d^3 r_N \quad (15')$$

In Born approximation one finds that the cross sections for the recoil distributions are proportional to $|V(\vec{q})|^2$ where $V(\vec{q})$ is the Fourier transform of $V(\vec{r})$

$$V(\vec{q}) = \frac{1}{(2\pi)^{3/2}} \int V(\vec{r}) e^{-i\vec{q} \cdot \vec{r}} d^3 r. \quad (16)$$

Inserting (15') one finds by elementary integration

$$\pm V_{oo}(\vec{q}) = -\sqrt{\frac{2}{\pi}} \sum \frac{e^2}{q_r^2} (1 - F(\vec{q})) \quad (17)$$

where

$$F(\vec{q}) = \frac{1}{Z} \int \Psi^*(\vec{r}_1, \dots, \vec{r}_N) \sum_j e^{-i\vec{q} \cdot \vec{r}_j} \Psi(\vec{r}_1, \dots, \vec{r}_N) d^3 r_1 \dots d^3 r_N \quad (18)$$

is called the atomic form factor, and $|1 - F(\vec{q})|^2$ is called the coherent scattering function. It can be computed when the wave function Ψ is known. For the Thomas-Fermi model it can be obtained in tabular form.⁴ The atomic form factor increases from zero proportional to q^2 for small q and approaches 1 asymptotically.

Because of the proportionality of the recoil distributions to $|V(\vec{q})|^2$ it follows immediately that screening is to be included by simply multiplying the unscreened recoil distributions by $|1 - F(\vec{q})|^2$. The other differential and total cross sections must then be obtained from the recoil distribution. This brings us to a discussion of the recoil distributions.

The Recoil Distributions

The computation of recoil distributions goes back to Bethe⁵ who needed them for precisely the same reason: the simplest way of including screening. The recoil distribution is a differential cross section in which the momentum transfer (\equiv recoil) is specified, i. e., it is of the form $\sigma(\vec{q}) d^3 q$. Since the form factor depends only on $|\vec{q}| = q$, we shall be content to compute $\sigma(q) dq$.

For this purpose it was observed by Bethe that it is essential to separate the problem into two parts, depending on the value of q , as follows:

Let $q_{\text{MIN}} \equiv \delta \ll \epsilon \ll m \ll q_{\text{MAX}}$. Then one defines a low q region $\delta \leq q \leq \epsilon$ in which the inequality $q \ll m$ is valid, such that higher powers of q/m can be neglected. One further defines a high q region, $\epsilon \leq q \leq q_{\text{MAX}}$ in which the inequality $\delta \ll q$ holds, such that powers of δ/q can be ignored. The quantity ϵ is otherwise arbitrary and eventually cancels from the final result. This cancellation comes about, because the low q region yields a result of the form

$$\sigma_L(q) = a(q) \ln \frac{\epsilon}{m} + b(q) \quad (19)$$

and the high q region yields

$$\sigma_H(q) = a(q) \ln \frac{m}{\epsilon} + c(q) \quad (20)$$

the total being $\sigma(q) = \sigma_L(q) + \sigma_H(q) = b(q) + c(q)$.

Multiplying $\sigma(q)$ by $|1 - F(q)|^2$ and integrating over q , Bethe finds the following differential cross sections. For pair production:

$$\sigma(E_+) dE_+ = 4\alpha r_0^2 Z^2 \frac{dE_+}{\omega^3} [(E_+^2 + E_-^2)(I_1 + 1) + \frac{2}{3} E_+ E_- (I_2 + \frac{5}{6})] ; \quad (21a)$$

for bremsstrahlung:

$$\sigma(\omega) d\omega = 4\alpha r_0^2 Z^2 \frac{d\omega}{\omega E^2} [(E^2 + E'^2)(I_1 + 1) - \frac{2}{3} E E' (I_2 + \frac{5}{6})] . \quad (21b)$$

The two integrals I_1 and I_2 are formally the same in both expressions,

$$I_1 = \int_{\delta}^m (1 - \frac{\delta}{q})^2 (1 - F(q))^2 \frac{dq}{q} \quad (22)$$

$$I_2 = \int_{\delta}^m (1 + 6(\frac{\delta}{q})^2) \ln \frac{\delta}{q} + 3(\frac{\delta}{q})^2 - 4(\frac{\delta}{q})^3 (1 - F(q))^2 \frac{dq}{q}$$

It will be important later on to recognize that the quantity $C(q)$ in (20) appears in (21) as the constants 1 and $5/6$ additive to the two integrals. Thus, the high q part contributes effectively relatively little to the cross section. Furthermore, it is not affected by the factor $(1 - F(q))^2$ i. e., it is independent of screening. This must be so, because large q means small b and therefore $b < a$.

A complete recoil distribution $\sigma(q)$ was computed by Jost, Luttinger, and Slotnick.⁶ We shall be content with equations (21), which yield the coherent cross sections.

The Coherent Cross Sections

Depending on the screening parameter γ (i. e. δ) one can now make various approximations in the evaluation of the integrals I_1 and I_2 . We shall discuss only the high energy limit ($\omega \gg m$ and $E \gg m$, respectively), which is most interesting for the majority of today's experiments and the only case where screening really matters.

Since the bremsstrahlung case, (21b), differs from that of pair production, (21a), essentially only by the sign of the factor $2/3$, we need to give here only the pair production case. Also, only the square bracket of (21) needs to be repeated. The following cases are important.

Case 1: no screening: $\gamma \gg 1$; actually $\gamma > 2$ often sufficiently accurate; $F(q) \sim 0$

$$[] = (E_+^2 + E_-^2 + \frac{2}{3} E_+ E_-) \left(\ln \frac{2E_+ E_-}{m\omega} - \frac{1}{2} \right) \quad (23)$$

Case 2: partial screening: $\gamma < 2$;

$$[] = (E_+^2 + E_-^2) \left(\frac{1}{4} \phi_1(\gamma) - \frac{1}{3} \ln Z \right) + \frac{2}{3} E_+ E_- \left(\frac{1}{4} \phi_2(\gamma) - \frac{1}{3} \ln Z \right) \quad (24)$$

The functions $\phi_1(\gamma)$ and $\phi_2(\gamma)$ are given in graphic form by Wheeler and Lamb⁷ and by Bethe and Ashkin.⁸

Case 3: complete screening: $\gamma \ll 1$, $\delta = 0$

$$I_1 = I_2 = \int_0^m (1 - F(q))^2 \frac{dq}{q} = \ln \frac{183}{Z^{1/3}} - 1 \quad (25)$$

$$[] = (E_+^2 + E_-^2 + \frac{2}{3} E_+ E_-) \ln \frac{183}{Z^{1/3}} - \frac{1}{9} E_+ E_- .$$

A fourth case, intermediate between our cases 1 and 2 is also given by Bethe and Ashkin.⁸

The total cross section arising from the complete screening case (25) is

$$\sigma_{\text{pair}} = \alpha r_0^2 Z^2 \left(\frac{28}{9} \ln \frac{183}{Z^{1/3}} - \frac{2}{27} \right)$$

which is to be compared with the unscreened cross section (11).

It is worth repeating that screening has to do with large impact parameters, i. e., small momentum transfers. The more the cross section depends on small q , the more will it be affected by screening. This situation is in contradistinction to the Coulomb corrections discussed previously. The Coulomb interaction is the larger the closer the incident (or outgoing) particle approaches the nucleus, i. e., the larger the momentum transfer q . It follows that the same Coulomb correction is applicable to all the different screening cases. The same function containing $f(Z)$, Eq. (12), is to be added to the square brackets (23) to (25). The resulting cross sections

$$\sigma_{\text{coh}}(E_+) dE_+ = 4\alpha r_0^2 Z^2 \frac{dE}{\omega^3} \left\{ [] + (E_+^2 + E_-^2 + \frac{2}{3} E_+ E_-) f(Z) \right\} \quad (26a)$$

and

$$\sigma_{\text{coh}}(\omega) d\omega = 4\alpha r_0^2 Z^2 \frac{d\omega}{\omega E^2} \left\{ [] + (E^2 + E'^2 - \frac{2}{3} EE') f(Z) \right\} \quad (26b)$$

then represent the coherent cross sections, corrected for screening (Eqs. (23) to (25)) and for the Coulomb interaction which is neglected in the Born approximation.

All the above screening corrections (23) to (25) are based on the Thomas-Fermi model. For light elements this is a poor model. In particular, for Hydrogen $F(q)$ can be computed exactly with the analytically known wave functions. The corresponding functions $\phi_i^{(n)}(r)$ and $\phi_i^{(n)}(r')$ needed in Eq. (24) are given by Wheeler and Lamb.⁷

Pair Production and Bremsstrahlung in the Field of a Free Electron

Before we consider our processes taking place with simultaneous excitation and ionization of the struck atom we must consider the simpler case of their occurrence in the field of a free electron (which actually is always a negaton). This process is, of course, also of interest on its own. In the pair production case it is sometimes known

as trident production, since one observes three characteristic prongs in emulsion or cloud chamber pictures.

The free electron case differs from the previously discussed nuclear case at first sight in two respects: There is an actual recoil whose energy is in general not negligible, and there is an exchange effect possible between the two negatons in the final state of pair production and in negaton bremsstrahlung. The latter case also contains two negatons in the initial state, but one of them is at rest and the other one has high energy, so that the exchange terms here are completely negligible. The reason for this will become clear a little later.

We shall first discuss pair production on free electrons. There will again be a threshold energy ω_{\min} . To compute it we note that in the center of the momentum system where $\vec{p} + \vec{p}' = 0$ (\vec{p} = momentum of initial electron) the minimum energy will be expended when the three electrons in the final state all are at rest (total energy $3m$). In the laboratory system, in which the initial electron is at rest, the final state therefore consists of three electrons (the pair and the recoil electron) all moving with the same velocity in the same direction (Fig. 6).

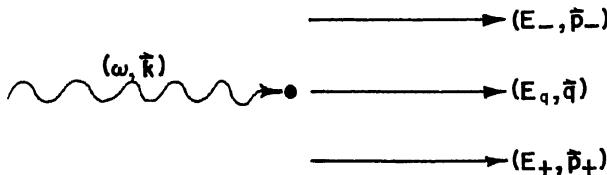


Fig. 6

Thus, at threshold, momentum conservation yields

$$\vec{p}_- = \vec{q} = \vec{p}_+ \quad \omega = 3q$$

and energy conservation yields

$$\omega + m = 3\sqrt{q^2 + m^2} = 3\sqrt{(\omega/3)^2 + m^2}$$

which can be solved for ω to yield the threshold energy in the laboratory system,

$$\omega = 4m, \quad (\text{Lab system}) \quad (27)$$

twice that for pair production in the nuclear field. In the center of momentum system this energy is

$$\omega = \frac{4}{3} m \quad (\text{C M-system}). \quad (28)$$

After a first estimate of the process by Perrin in 1934 and various limiting cases discussed by Watson, Nemirovsky, and others, Borsellino in 1947 made the first serious calculation of this process. However, he made a computation of a somewhat different process which, when applied to our case is seriously modified by various simplifying assumptions of which we only want to mention that of the neglect of exchange. A detailed discussion of these earlier papers is to be found in the review article.¹

In 1948 Votruba made the first quantum electrodynamic calculation which is exact and consistent to the lowest non-vanishing order of perturbation theory; it is again essentially a Born approximation. However, he could not carry through the general calculations to the final results, because of their extreme complexity (relativistic third order perturbation theory!). He computed cross sections only for limiting cases. His results are as follows: Near threshold ($\omega - 4m \ll m$):

$$\sigma = \alpha r_e^2 \frac{\pi\sqrt{3}}{2^2 3^5} \left(\frac{\omega}{m} - 4 \right)^2 ; \quad (29)$$

at very high energy:

(I) when one of the final negatons is slow ($q \ll m$), the other one and the positon is fast,

$$\sigma_I = \alpha r_e^2 \left(\frac{28}{q} \ln \frac{2\omega}{m} - \frac{102 \pm 4}{q} \right) ; \quad (30)$$

(II) when the positon is slow and both final negatons are fast,

$$\sigma_{II} = \alpha r_e^2 \cdot \frac{2}{3} \ln \frac{\omega}{m} / \frac{\omega}{m} ; \quad (31)$$

(III) when all three final electrons are fast,

$$\sigma_{III} \sim \alpha r_e^2 \cdot \frac{1}{50} . \quad (32)$$

These results should first of all be compared with the Bethe-Heitler results for $Z = 1$. Near threshold (compare (29) with (10)) the cross section increases like a parabola of second degree (rather than third degree) and has a much smaller coefficient. Both contributing to a much slower rise of the electron case as compared to the nuclear case. Of course,

the Coulomb corrections are largest near threshold and may modify (29) very essentially (just as is the case for (10)).

At very high energies large impact parameters play an increasingly important role. Thus, most collisions will take place with very small momentum transfer q . The struck electron then receives only a small "side-kick," a glancing collision. In that case the recoil q is so small that the cross section is practically independent of the mass of the recoiling particle, which then might as well be a nucleus. Thus, at very high energy and for small momentum transfers, the electron case and the nuclear case with $Z = 1$ should give identical cross sections.

This is indeed seen to be the case on comparing (30) with (11): The logarithmic terms (which are the leading terms) are the same. The constant terms are not quite the same, although they are not very different from each other. Votruba's $(102\pi^4)/q$ was based on an estimate of a certain integral. It has since been possible to carry out this integration exactly¹ with the result

$$\Omega_I = \alpha r^2 \left(\frac{28}{q} \ln \frac{2\omega}{m} - \frac{100}{q} \right) : \quad (33)$$

Neglecting Ω_{II} and Ω_{III} , we can identify Ω_I with the total pair production cross section in the field of a free electron. Eq. (33) is then smaller than the Bethe-Heitler formula with $Z = 1$, (Eq. (11)), by

$$\Delta\sigma = \alpha r_0^2 \cdot \frac{87}{27} . \quad (34)$$

The physical interpretation of this difference is apparently that it is due to exchange. However, let us first take a closer look at Votruba's derivation of (30). Could the difference (34) be due to an approximation in the derivation of (30)?

Let us recall Bethe's derivation of the recoil distribution which yielded the basic formulae (21). There the separation by a quantity $\epsilon \ll m$ into low q and high q parts was essential. If we try to repeat this procedure in the electron case we see that the low q part is identical with Ω_I , but with an upper cut-off ϵ (rather than m , as Votruba assumed!); the high q part, however, is not the same as Ω_{II} , because it needs the assumption $q \gg \delta$, whereas Votruba assumed $q \gg m$ which is stronger. Thus, $\Omega_I + \Omega_{II}$ involves a region $q \leq m$ which is poorly approximated. It is included to some extent in Ω_I by choosing the upper cut-off to be m rather than ϵ .

Let us now compare Ω_I with the low q part of the nuclear cross section, cut off at $\epsilon = m$. Thus, we compare Ω_I with $b(q)$ in (19). But $b(q) + c(q)$ is given in (21) and $c(q)$ gives just the terms involving 1 and $5/6$. Therefore, $b(q)$ differs from the nuclear cross section with $Z = 1$ exactly by

$$4\alpha r_0^2 \int \frac{dE}{\omega^3} \left[(E_+^2 + E_-^2) \cdot 1 + \frac{2}{3} E_+ E_- \cdot \frac{5}{6} \right] = \alpha r_0^2 \frac{82}{27} \quad (35)$$

This is identical with (34), which means that

$$\int_{-\infty}^{\infty} b(q) dq = \sigma_I. \quad (36)$$

We conclude from this result that in the high energy limit any difference between the nuclear and the electron case lies entirely in the high q part. This is not surprising for the most important physical difference, the exchange effect: It arises when the two negatons in the final state are close enough in phase space to invoke the Pauli exclusion principle. Clearly, this will happen only when they have comparable energies. σ_I will therefore not be affected by exchange, and only large recoil cases will show an exchange effect.

A further comparison between the electron and the nuclear case indicates that $\sigma_I + \sigma_W$ is probably a pretty good estimate of the free electron case and certainly a lower limit. This means that most of the high q part is suppressed by exchange. (Cf. the more detailed discussion on this point in the review article.)

We can summarize the high energy calculations by saying that for pair production in the field of an electron the Bethe-Heitler cross sections with $Z = 1$ are definitely an overestimate. The Votruba result yields an underestimate, but it is most likely closer to the correct value.

It then follows further that the Bethe-Heitler low q recoil distribution for $Z = 1$ is a fairly good approximation to the recoil distribution of a free electron due to pair production. This recoil distribution was found to be of the form

$$\sigma(\omega, q) dq = 4\alpha r_0^2 \frac{\omega}{m} f\left(\frac{q\omega}{2m^2}\right) \frac{dq}{m}; \quad (37)$$

the function f is given in the review article. Note that q enters only in the form $\frac{q\omega}{2m^2}$.

The arguments and results presented so far for pair production

in the field of a free electron are mutatis mutandis also valid for bremsstrahlung in the field of a free electron. The calculation analogous to Votruba's work was done by Hodes,⁹ but was not carried equally far. Here, the substitution law is of great help and permits us to draw many conclusions from the pair production case. However, we shall not discuss bremsstrahlung by free electrons any further.

It remains to emphasize that we know nothing about Coulomb corrections for either pair production or bremsstrahlung in the electron field. This is particularly unfortunate in the energy region of beta-rays where many important experiments are being done and where these corrections may be quite large.

The Incoherent Scattering Function

We now return to the case where our processes are taking place in the field of the atom as a whole. How can we describe them when they occur with a simultaneous excitation or ionization of the atom?

When we consider Fig. 3 and Eq. (7) for the matrix element M_{fi} , we see that the difference between the stripped atom (nucleus) and the actual atom lies in the matrix elements of H_{ext} . For the stripped atom H_{ext} is the interaction between the incident electron and the nucleus; for the actual atom it is the interaction between the incident electron and the whole atom, i. e., the nucleus and the atomic electrons which in turn interact with the nucleus. This latter interaction need not be taken into account explicitly; it is implied in the initial and final wave functions for the whole atom, $\Psi_i(\vec{r}_1, \dots, \vec{r}_N)$ and $\Psi_f(\vec{r}_1, \dots, \vec{r}_N)$. Since H_1 will not change the state of the atom, it then follows from (7) that the matrix elements of H_{ext} must be generalized to include the transition

$\Psi_i \rightarrow \Psi_f$ of the electron cloud. Effectively, therefore, we must make the replacement

$$\mp H_{ext} = e \phi_{ext} = \frac{ze^2}{r} \longrightarrow$$

$$\mp H_{ext} = \int \Psi_f^*(\vec{r}_1, \dots, \vec{r}_N) \left[\frac{ze^2}{r} - \sum_{j=1}^N \frac{e^2}{|\vec{r} - \vec{r}_j|} \right] \Psi_i(\vec{r}_1, \dots, \vec{r}_N) d^3r_1 \dots d^3r_N. \quad (38)$$

Since $\Psi_i = \Psi_0$, the ground state of the atom, we have for $\Psi_f = \Psi$

$$H_{ext} = V_{oo}(\vec{r}) \quad (39)$$

with $V_{oo}(\vec{r})$ given by (15'). But when $\Psi_f \neq \Psi_i$ the first term in (38) vanishes because of the orthogonality of the wave functions, and the remainder yields

$$H_{\text{EXT}} = V_{f_0}(\vec{r}) = - \int \Psi_f^*(\tau) \sum_{i=1}^N \frac{e^2}{|\vec{r} - \vec{r}_i|} \Psi_o(\tau) d\tau \quad (40)$$

Taking the Fourier transform,

$$V_{f_0}(q) = - \sqrt{\frac{2}{\pi}} \frac{e^2}{q^2} \sum_{i=1}^N \int \Psi_f^*(\tau) e^{-i\vec{q} \cdot \vec{r}_i} \Psi_o(\tau) d\tau . \quad (41)$$

This expression appears as a factor in the recoil distribution amplitude. The recoil distribution cross section for pair production or bremsstrahlung which leaves the atom in any state f different from o is therefore proportional to

$$\begin{aligned} \sum_{f \neq o} |V_{f_0}(q)|^2 &= \frac{2}{\pi} \left(\frac{e^2}{q^2} \right)^2 S(q) \\ S(q) &= \sum_f \sum_{i,j} \int \Psi_o^*(\tau) e^{i\vec{q} \cdot \vec{r}_i} \Psi_f(\tau) d\tau \cdot \int \Psi_f^*(\tau') e^{-i\vec{q} \cdot \vec{r}_j} \Psi_o(\tau') d\tau' \\ &= \sum_{i,j} \int \Psi_o^*(\tau) e^{i\vec{q} \cdot \vec{r}_i} d\tau [\delta(\tau - \tau') - \Psi_o(\tau) \Psi_o^*(\tau')] e^{-i\vec{q} \cdot \vec{r}_j} \Psi_o(\tau') d\tau' \\ &= \sum_{i,j} \int \Psi_o^*(\tau) e^{i(\vec{q} \cdot \vec{r}_i - \vec{r}_j)} \Psi_o(\tau) d\tau - \left| \sum_j \int \Psi_o^*(\tau) e^{i\vec{q} \cdot \vec{r}_j} \Psi_o(\tau) d\tau \right|^2 \end{aligned} \quad (42)$$

Here we used the completeness relation for the complete set of functions

$$\Psi_o, \Psi_i, \dots .$$

The quantity $S(q)$ is called the incoherent scattering function. It plays the same role for incoherent scattering as the coherent scattering function plays for coherent scattering. It also has the same qualitative behavior. Note that relation (17) emerges naturally as a special case from our more general considerations (38).

$S(q)$ has been evaluated numerically for Thomas-Fermi wave functions¹⁰ and for Hartree wave functions.¹¹ It can be obtained analytically for Hydrogen, where it is simply

$$S(q) = 1 - |Q_o(q)|^2 = 1 - \left[\frac{1}{1 + (q/2\alpha m)^2} \right]^4 \quad (43)$$

$$Q_o(\vec{r}) = \Psi_o^*(\vec{r}) \Psi_o(\vec{r}).$$

The Incoherent Cross Sections

These cross sections, just as the coherent ones, follow from the recoil distribution (momentum transfer distributions). Here, however, it is the momentum transfer to the individual bound atomic electrons, rather than to the nucleus. Not knowing this distribution, we can approximate it either by the momentum transfer distribution to the nucleus or by the momentum transfer distribution to a free electron. Wheeler and Lamb⁷ used the former; Dr. Joseph and I proposed the latter.¹ Even this latter distribution, however, does not describe the situation exactly. We shall refer the corrections to it as binding energy corrections.

In the approximation adopted by Wheeler and Lamb the cross sections (21) are used with $Z = 1$ and with $(1 - F(q))^2$ replaced by $S(q)$ in the integrals (22). In analogy with (24) they obtained (multiplying by Z for the Z independently acting atomic electrons) for pair production

$$\begin{aligned} \sigma_{\text{INCOH}}(E_+) dE_+ &= 4 \alpha r_o^2 Z \frac{dE_+}{\omega E^2} \left[(E_+^2 + E_-^2) \left(\frac{1}{4} \Psi_1(\epsilon) - \frac{2}{3} \ln Z \right) \right. \\ &\quad \left. + \frac{2}{3} E_+ E_- \left(\frac{1}{4} \Psi_2(\epsilon) - \frac{2}{3} \ln Z \right) \right] \end{aligned} \quad (44a)$$

and for bremsstrahlung,

$$\begin{aligned} \sigma_{\text{INCOH}}(\omega) d\omega &= 4 \alpha r_o^2 Z \frac{d\omega}{\omega E^2} \left[(E^2 + E'^2) \left(\frac{1}{4} \Psi_1(\epsilon) - \frac{2}{3} \ln Z \right) \right. \\ &\quad \left. - \frac{2}{3} E E' \left(\frac{1}{4} \Psi_2(\epsilon) - \frac{2}{3} \ln Z \right) \right]. \end{aligned} \quad (44b)$$

The functions $\Psi_1(\epsilon)$ and $\Psi_2(\epsilon)$ arise from the Thomas - Fermi wave functions in $S(q)$ which makes $S(q)$ depend only on the combination

$$\gamma = \sqrt[3]{6\pi} \frac{q/m}{8\alpha} \frac{1}{Z} . \quad (45)$$

Integrating over q between $\delta_1 = \delta(Z=1)$ and m then yields a function which, from the upper limit, depends only on $Z^{2/3}$ yielding the term $\frac{5}{3} \ln Z$, and which, from the lower limit, depends only on

$$\frac{\sqrt[3]{6\pi}}{8\alpha} \cdot \frac{\delta_1/m}{Z^{2/3}} = \frac{\sqrt[3]{6\pi}}{8\alpha} \frac{1}{Z^{2/3}} \cdot \begin{cases} \frac{m\omega}{2E_+ E_-} \\ \frac{m\omega}{2EE'} \end{cases} = \frac{\sqrt[3]{6\pi}}{1600\alpha} \epsilon \quad (46)$$

with

$$\epsilon = \frac{100}{Z^{2/3}} \cdot \frac{m\omega}{E_+ E_-} \quad \text{for pair production} \quad (47)$$

$$\epsilon = \frac{100}{Z^{2/3}} \cdot \frac{m\omega}{EE'} \quad \text{for bremsstrahlung}$$

Thus, ϵ is a convenient parameter characterizing the incoherent processes¹² and is simply related to the screening parameter γ (14). The functions $\psi(\epsilon)$ and $\psi_2(\epsilon)$ are given graphically in reference (7).

In the limit $\epsilon \rightarrow 0$ ("complete incoherence") which, in a sense, corresponds to complete screening in the coherent case, (44) reduces to

$$\sigma_{\text{incoh}}(E_+) dE_+ = 4\alpha r_0^2 Z \frac{dE_+}{\omega^3} [E_+^2 + E_-^2 + \frac{2}{3} E_+ E_-] \ln \left[\frac{1440}{Z^{2/3}} - \frac{1}{q} E_+ E_- \right] \quad (48a)$$

$$\sigma_{\text{INCOH}}(\omega) d\omega = 4\alpha r_o^2 Z \frac{d\omega}{\omega E^2} \left[(E^2 + E'^2 - \frac{2}{3} EE') \ln \frac{1440}{Z^{2/3}} + \frac{1}{q} EE' \right] \quad (48b)$$

Eq. (48a) yields the total cross section

$$\sigma_{\text{INCOH}} = \alpha r_o^2 Z \left(\frac{28}{9} \ln \frac{1440}{Z^{2/3}} - \frac{2}{27} \right). \quad (49)$$

These are the results obtained by approximating the bound electron recoil distribution by the nuclear recoil distribution (infinite mass - es). If, on the other hand, we want to approximate it by the free electron distribution we can simply argue as follows. The nuclear and the free electron distribution differ at high energies only by the exchange terms (cf. eq. (35)). These arise from the high q part which does not depend on screening in the coherent case and therefore also not on $S(q)$ in the incoherent case. They are thus independent of ϵ . This fact is obviously a consequence of the connection of exchange with large momentum transfers and of screening with small momentum transfers.

It follows that the exchange correction is independent of ϵ and is simply the quantity (34) times Z . This must be subtracted from the Wheeler-Lamb cross sections (44) and (48),

$$\Delta\sigma_{\text{EXCH}}(E) dE = 4\alpha r_o^2 Z \frac{dE}{\omega^3} \left(E_+^2 + E_-^2 + \frac{5}{q} E_+ E_- \right) \quad (50a)$$

$$\Delta\sigma_{\text{EXCH}}(\omega) d\omega = 4\alpha r_o^2 Z \frac{d\omega}{\omega E^2} \left(E^2 + E'^2 - \frac{5}{q} EE' \right). \quad (50b)$$

In the $\epsilon \rightarrow 0$ limit (48) then becomes

$$\sigma_{\text{INCOH}}^{\text{EXCH}}(E_+) dE_+ = 4\alpha r_o^2 Z \frac{dE_+}{\omega^3} \left(E_+^2 + E_-^2 + \frac{2}{3} E_+ E_- \right) \ln \frac{530}{Z^{2/3}} \quad (51a)$$

$$\sigma_{\text{INCOH}}^{\text{EXCH}}(\omega) d\omega = 4\alpha r_o^2 Z \frac{d\omega}{\omega E^2} \left(E^2 + E'^2 - \frac{2}{3} EE' \right) \ln \frac{530}{Z^{2/3}} \quad (51b)$$

and Eq. (49), the total pair production cross section, reads

$$\sigma_{\text{INCOH}}^{\text{EXCH}} = \alpha r_o^2 Z \cdot \frac{28}{9} \ln \frac{530}{Z^{2/3}} . \quad (52)$$

The case of Hydrogen deserves again separate consideration, because the above relations based on the Thomas-Fermi model are not applicable. The incoherent scattering function (43) can be integrated numerically with the Bethe-Heitler recoil distribution yielding the Wheeler-Lamb result (44) with $Z = 1$ and $\Psi_1(\epsilon)$ and $\Psi_2(\epsilon)$ replaced by $\Psi_1^{(H)}(\epsilon)$ and $\Psi_2^{(H)}(\epsilon)$ which are also given graphically by these authors. The limit can be obtained analytically, yielding Eqs. (48) and (49) with the replacement

$$\ln \frac{1440}{Z^{2/3}} \rightarrow \ln \frac{1}{2\alpha} + \frac{23}{12} \quad (53)$$

and $Z = 1$. The exchange correction is of course the same as before, i. e. (50) with $Z = 1$. In particular, the total incoherent pair production cross section in Hydrogen including exchange and in the limit $\epsilon \rightarrow 0$ becomes

$$\sigma_{\text{INCOH}}^{(H)\text{EXCH}} = \alpha r_o^2 \frac{28}{9} \left(\ln \frac{1}{2\alpha} + \frac{11}{12} \right) = 16.0 \alpha r_o^2 . \quad (54)$$

Due to exchange, this cross section is 17 percent smaller than the Wheeler-Lamb value.

The Present State of the Theory

The calculation of pair production and bremsstrahlung on atoms in its various successive approximations may be summarized as follows:

(a) The Born approximation for the stripped atom; this is proportional to Z^2 and gives the bulk of the cross sections (Bethe-Heitler formulae).

(b) The Coulomb corrections to (a); these are known for high energies.

(c) The radiative corrections to (a); these are small, of order α .

(d) The screening corrections to (a); these are important at high energies.

The sum of (a) to (d) yields the coherent cross sections.

(e) The incoherent cross sections in Born approximation neglecting exchange; these are proportional to Z . (Wheeler-Lamb)

(f) Corrections to the incoherent scattering function.

(g) The exchange and recoil corrections to (e).

(h) The binding energy correction to (e).

The sum of (a) to (f) gives the complete theoretical cross sections.

This enumeration shows clearly the holes still existing in our present theoretical knowledge. Only (a) and (e) are completely known. But unless the energies are high the Born approximations are poor.

(b) is not known where it is largest, i. e., in the energy region of betarays, and (c) is completely unknown. (d) is known only for Thomas-Fermi wave functions. Accurate measurements on light elements and at high energies require better wave functions. The same remark holds for (f) since the incoherent scattering function usually used is also based on the Thomas-Fermi model. But the incoherent cross sections are largest for light elements where this model is poor. (g) is known only in an overestimate. Finally, the binding energy correction (h) to (a) is again completely unknown. It may be an important correction, especially for the lower energy region.

A different type of insufficiency of our theory is the detail with which these cross sections are known. The total cross sections are better known than the differential cross sections. Nothing is known, e. g. about the angular distributions of the incoherent cross sections. Even the incoherent recoil distribution is known only for free electrons and $q \ll m$. Further detail concerns the polarization of the photon and the spin orientation of the electrons. These are known only in approximation (a). We do not know, e. g., how the Coulomb corrections affect them.

It is very difficult to distinguish experimentally between the coherent and incoherent events. All excitations are incoherent, but cannot be distinguished experimentally from the coherent events. The same

holds for ionizations with electron recoils too small to be seen. Thus, in general it will be better to draw a line at the smallest still observable recoil q_e and measure $\sigma_{\text{INCOH}}(q_e > q_e)$ and $\sigma_{\text{coh}} + \sigma_{\text{INCOH}}(q_e < q_e)$. This complicates comparison with theory at the present time, because $\sigma_{\text{INCOH}}(q_e \geq m)$ is almost completely unknown theoretically.

When we now compare our best calculations with some recent experiments all these weak points must be kept in mind. I cannot emphasize enough the importance of a very careful comparison of experimental results with the theory. The various approximations must be taken for what they are and not for exact theory. Thus, if an experiment agrees with the Born approximation (a) to very high accuracy, this is not a confirmation of theory. It only shows that the corrections (b) through (h) -- some of which being only poorly known or unknown -- add to zero. Or, if one wants to establish the experimental value for the exchange correction (g), one can do so only within the error to which all the other corrections are known. For this reason the following experiments will be given with little or no comment. Each would require careful error estimates.

Some Recent Experiments

Consider now some recent experiments. An experiment on pair production by Ch. Frei (private communication) at .6.3 Mev gave a value of 0.50 ± 0.05 for the ratio of $\frac{\sigma}{\sigma_{\text{coh}}}$ where the total cross section is assumed to be of the form $\sigma = Z^2 \frac{\sigma}{\sigma_{\text{coh}}} + Z \frac{\sigma}{\sigma_{\text{coh}}}$. If this is compared to the ratio $Z \frac{\sigma_{\text{INCOH}}}{\sigma_{\text{coh}}}/\sigma_{\text{coh}}$ one finds a theoretical value of 0.14. This value does not include the complete corrections (g) which might increase it, but can hardly be expected to change it by a factor of more than 3. Since the actual cross section is of a much more complicated Z dependence, it is not clear whether the observed ratio should be identified with $Z \frac{\sigma_{\text{INCOH}}}{\sigma_{\text{coh}}}/\sigma_{\text{coh}}$. Also, (h) may play an important role here.

Another experiment, at 319 Mev photon energy¹³ yields the following values on H and C for σ_{INCOH} which are compared with the approximations (e) and (e) + (g) (all values in mb):

	(e)	exp	(e) + (g)
H	8.05	6.8 ± 1.8	6.29
C	46.7	46.6 ± 6.8	36.1

The approximation (e) and (e) + (g) are over and underestimates, respectively. However, the theoretical values for C are poor since the Thomas-Fermi model is poor for C.

Recent experiments by Hart and Cocconi yield experimental momentum and angular distributions of the recoil electron in triplet production.

The theoretical data are very meager on these points, especially for $q \geq m$ and much more theoretical work is needed to make full use of these data.

Moffatt (private communication) recently measured pair production in Hydrogen and obtained the incoherent cross sections shown in Fig. 7. The upper curve, marked "Borsellino," is below the nuclear pair cross section for $Z = 1$. Since $\epsilon > 2$ these curves are practically the same as the cross sections in the field of a free electron.

EXPERIMENTS BY MOFFATT (OXFORD)

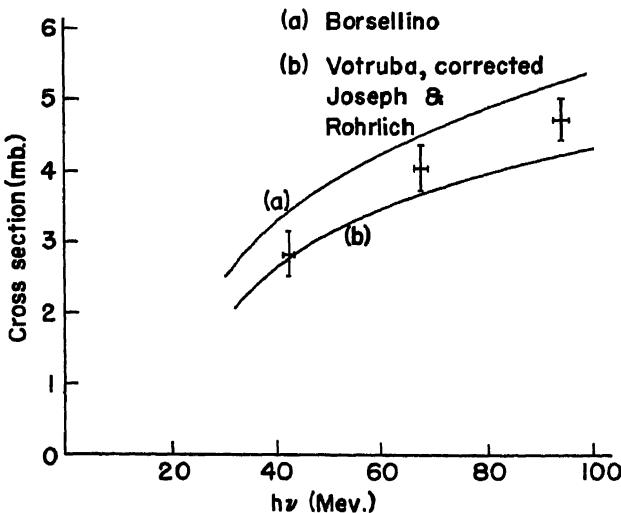


Fig. 7 Cross section for pair production on free electron.
(standard errors are shown for experimental data)

A bremsstrahlung experiment by Bernstein and Panofsky¹⁴ with 500 and 550 Mev electrons on molecular Hydrogen yielded after suitable subtractions a value for the exchange term of 5.1 ± 2.8 percent of the total cross section. The (over) estimate (g) yields 9.4 percent.

All these observations show that more as well as more accurate measurements are needed to check on those theoretical results which are presently available; and that more as well as more accurate computations are needed to check on those experiments whose interpretation is so far beyond our theoretical knowledge.

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THEORY OF PARTICLES WITH ZERO REST-MASS*

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I. Introduction

Recently a new point of view has been found which applies to non-interacting particles of zero rest-mass and which gives for them a wave equation, transformation properties, and formulas for energy, momentum, and angular momentum in remarkable parallel to Dirac's theory of the electron. The purpose of these lectures is to give some of the details of this new point of view.

One can make a uniform treatment for spins greater than zero, integral or half-integral. The spin 1/2 specialization is the two-component neutrino theory and the spin 1 specialization is Maxwell's theory for the photon. As is well known, 1,2 free particles with discrete spin and zero rest-mass only exist in two states, spin parallel or anti-parallel to the momentum, so one discusses here a screwon of arbitrary spin. For the photon these two states are of circular polarization, right/left hand circularly polarized with the propagation direction for spin parallel/antiparallel to the momentum.

The wave equations themselves are

$$H\phi = i\hbar \partial_t \phi , \quad (1)$$

where

$$H = (\frac{c}{\lambda}) \vec{P} \cdot \vec{\Delta} , \quad (2)$$

$$\vec{P} = -i\hbar \nabla ,$$

$\vec{\Delta}$ are the angular momentum matrices for spin s (factor \hbar not included), and ϕ is a $2s+1$ component wave function written as a column matrix. These equations have more than the two solutions and are not alone covariant by Lorentz transformations (except for the spin 1/2

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specialization). They must be supplemented by the auxiliary condition that only the solutions with spins parallel or antiparallel to the momentum are retained and the wave equation plus this auxiliary condition makes a covariant statement.

The wave equation and auxiliary condition are equivalent to the Dirac-Pauli-Fierz³ system of equations for zero rest-mass. This system of equations applies to any spinor quantity that has the dispersion $\omega^2 = c^2 p^2$ so it is perhaps the most general system that ever need be considered. The point of view considered here replaces the redundant spinor components by a column matrix of independent elements and the spinor operations by ordinary matrix multiplication so that a more fluent discussion of the equations can be made.

A distinction is made between the spinor components of the field ψ which transform linearly with respect to Lorentz transformations and the wave function components ϕ which are used to form the energy, momentum, and angular momentum of the field as expectation values of the displacement operators. The relation between them is

$$\psi = |\mathcal{H}/c|^{1/2} \phi \quad (3)$$

so it is clear that ϕ will not transform linearly and it is not a spinor; this is perhaps why this type of theory was not considered before. However, ϕ is defined in every Lorentz frame by this relation with ψ so its transformations do represent the Lorentz group.

The two states have eigenvalues $\pm c\mathcal{P}$ of \mathcal{H} . For integral spin the particles are Bosons so one cannot interpret \mathcal{H} as the energy and apply a hole theory as Dirac does for the electron. However, one can assign

$$|\mathcal{H}|, (\mathcal{H}/|\mathcal{H}|)\vec{P}, (\mathcal{H}/|\mathcal{H}|)(\vec{x} \times \vec{P} + \hbar \vec{\Delta})$$

to be the energy, momentum, and angular momentum operators. This avoids all the difficulties and is equivalent to the hole theory for half-integral spin.

The fact that Maxwell's equations can be written as a particle type of wave equation permits them to be studied using standard quantum mechanical methods. In particular the problem of finding the multipole radiation patterns from a point source can be worked out very easily in parallel with the Schrödinger or Dirac radial problems, making use of the fact that the angular momentum operators commute with the Hamiltonian. The interesting result is that the well-known multipole radiation patterns are eigenfunctions of the angular momentum and space-reflection operators for the electromagnetic field.

The quantization process for the theory can be carried out in a

straightforward way and it leads to a simple and direct connection between the spin and the statistics of the particles. It is found that the spinor components of a Boson/Fermion field with integral/half-integral spin commute/anticommute off the light cone whereas the spinor components of a Boson/Fermion field with half-integral/integral spin do not.

Section II below gives a summary of some of the pertinent properties of the two-component neutrino theory and the rest of the sections treat, in order, the photon, the multipole radiation problem, the general theory for arbitrary spin, and the quantization. The work on the particle aspect of Maxwell's theory and multipole radiation was done mainly at Department of Physics, Pennsylvania State University; that on the theory for arbitrary spin and its quantization was done in collaboration with C. L. Hammer at Physics Department and Institute for Atomic Research, Iowa State College.

II. The Two-Component Neutrino

The two-component neutrino theory was originally discovered by Weyl.⁴ When, as suggested by Lee and Yang,⁵ the experiment of Wu, Ambler, Hayward, Hoppes, and Hudson⁶ showed that parity was not conserved in beta decay, Landau,⁷ Lee and Yang,⁸ and Salam⁹ proposed that it was a two-component neutrino emitted in the beta transition. Since that time there have been so many experimental confirmations of this idea that the existence of the two-component neutrino seems established. Especially the beta decay reaction proposed by Feynman and Gell-Mann,¹⁰ Marshak and Sudarshan,¹¹ and Sakurai¹² is now in almost complete agreement with experiment.

The wave equation for the two-component neutrino is

$$H\psi = i\hbar \frac{\partial}{\partial t} \psi ,$$

where

$$H = c \vec{p} \cdot \vec{\sigma} , \quad (4)$$

and $\vec{\sigma}$ are the Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} , \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} , \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} .$$

The covariance of the equation with respect to continuous Lorentz transformations

$$X'_\alpha = \alpha_{\alpha\beta} X_\beta$$

(α_4 is ict) can be easily demonstrated by using the notation

$$\tilde{\sigma}_4 = i ,$$

$$p_4 = -i\hbar \frac{\partial}{\partial x_4} = -\hbar c^{-1} \frac{\partial}{\partial t}$$

so that the equation takes the form

$$p_\mu \tilde{\sigma}_\mu \psi(x) = 0 . \quad (5)$$

The equation will have the same form in the primed coordinate system

$$p'_\mu \tilde{\sigma}'_\mu \psi'(x') = 0$$

if the wave function transforms according to

$$\psi'(x') = \Lambda \psi(x) \quad (6)$$

where the matrix Λ satisfies the equation

$$\Lambda^H \tilde{\sigma}_\alpha \Lambda = \alpha_{\alpha\beta} \tilde{\sigma}_\beta . \quad (7)$$

Such a matrix Λ can be found and in fact one solution (which will be used here throughout) has the form

$$\Lambda = \exp(i\vec{\beta} \cdot \vec{\sigma}/2) \quad (8)$$

where $\vec{\beta}$ is a three-vector with complex components, corresponding to the six parameters of the Lorentz group. To see the truth of this statement one considers the cases of real $\vec{\beta}$ and pure imaginary $\vec{\beta}$ separately. The multiplication rules for the Pauli matrices,

$$\tilde{\sigma}_i \tilde{\sigma}_j = i \epsilon_{ijk} \tilde{\sigma}_k + \delta_{ij} , \quad (9)$$

imply that

$$(\vec{\beta} \cdot \vec{\sigma})^2 = \beta_i \tilde{\sigma}_i \beta_j \tilde{\sigma}_j$$

$$= \beta_i \beta_i$$

so that the exponential function simplifies as follows:

$$\begin{aligned} \exp(i\frac{1}{2}\vec{\beta} \cdot \vec{\sigma}) &= \sum_{n=0}^{\infty} \frac{(i\frac{1}{2}\vec{\beta} \cdot \vec{\sigma})^n}{n!} \\ &= \sum_{\text{even } n} \frac{(i\frac{1}{2}\beta)^n}{n!} + i\frac{\vec{\beta} \cdot \vec{\sigma}}{\beta} \sum_{\text{odd } n} \frac{(i\frac{1}{2}\beta)^n}{n!} \\ &= \cos \frac{1}{2}\beta + i\beta^{-1} \vec{\beta} \cdot \vec{\sigma} \sin \frac{1}{2}\beta, \end{aligned}$$

where β is defined to have argument 0 or $\pi/2$. Then for real $\vec{\beta}$ Eq. (7) becomes

$$\begin{aligned} \alpha_{\beta} \sigma_{\beta} &= (\cos \frac{1}{2}\beta - i\beta^{-1} \vec{\beta} \cdot \vec{\sigma} \sin \frac{1}{2}\beta) \alpha_{\beta} \\ &\quad (\cos \frac{1}{2}\beta + i\beta^{-1} \vec{\beta} \cdot \vec{\sigma} \sin \frac{1}{2}\beta), \end{aligned}$$

$$\alpha_{4\beta} \sigma_{\beta} = \sigma_4,$$

$$\begin{aligned} \alpha_{i\beta} \sigma_{\beta} &= (\cos^2 \frac{1}{2}\beta) \alpha_i + \beta^{-2} \vec{\beta} \cdot \vec{\sigma} \sigma_i \vec{\beta} \cdot \vec{\sigma} \sin^2 \frac{1}{2}\beta \\ &\quad + i\beta^{-1} (\cos \frac{1}{2}\beta) (\sin \frac{1}{2}\beta) (\sigma_i \vec{\beta} \cdot \vec{\sigma} - \vec{\beta} \cdot \vec{\sigma} \sigma_i). \end{aligned}$$

One simplifies the second term easily by using

$$\sigma_i \sigma_j + \sigma_j \sigma_i = 2 \delta_{ij}$$

and the third by using Eq. (9):

$$\begin{aligned}
 \alpha_{ij} \alpha_{il} &= \cos^2 \frac{1}{2}\beta \alpha_i - \sin^2 \frac{1}{2}\beta \alpha_i \\
 &\quad + 2\beta^{-2} \beta_i \vec{\beta} \cdot \vec{\sigma} \sin^2 \frac{1}{2}\beta \\
 &\quad + 2i\beta^{-1} \cos \frac{1}{2}\beta \sin \frac{1}{2}\beta i \epsilon_{ijk} \beta_j \alpha_k \\
 &= \cos \beta \alpha_i + \epsilon_{ijk} \beta_k \alpha_j \beta^{-1} \sin \beta \\
 &\quad + \beta_i \vec{\beta} \cdot \vec{\sigma} \beta^{-2} (1 - \cos \beta).
 \end{aligned}$$

It is seen that when β is real Eq. (7) is satisfied and the transformation coefficients are

$$\begin{aligned}
 \alpha_{ii} &= \delta_{ij} \cos \beta + \epsilon_{ijk} \beta_k \beta^{-1} \sin \beta + \beta_i \beta_j \beta^{-2} (1 - \cos \beta), \\
 \alpha_{i4} &= \alpha_{4i} = 0, \tag{10}
 \end{aligned}$$

$$\alpha_{44} = 1.$$

This is a space rotation because the α_{ij} form an orthogonal matrix:

$$\begin{aligned}
 \alpha_{ij} \alpha_{il} &= \delta_{ij} \cos^2 \beta + \epsilon_{ijk} \beta_k \beta^{-1} \sin \beta \cos \beta \\
 &\quad + \beta_i \beta_j \beta^{-2} \cos \beta (1 - \cos \beta) + \epsilon_{jlm} \beta_m \beta^{-1} \sin \beta \cos \beta \\
 &\quad + \epsilon_{ijk} \epsilon_{ilm} \beta_k \beta_m \beta^{-2} \sin^2 \beta \\
 &\quad + \beta_i \beta_j \beta^{-2} \epsilon_{ilm} \beta_m \beta^{-1} \sin \beta (1 - \cos \beta)
 \end{aligned}$$

$$+\beta_i \beta_j \beta^{-2} \cos \beta (1 - \cos \beta) \\ + \epsilon_{ijk} \beta_k \beta_i \beta_j \beta^{-3} \sin \beta (1 - \cos \beta) + \beta_j \beta_k \beta^{-2} (1 - \cos \beta)^2$$

$$\alpha_{ij} \alpha_{ij} = \delta_{ij} \cos^2 \beta + \delta_{jk} \sin^2 \beta \\ + \beta_i \beta_j \beta^{-2} (2 \cos \beta - 2 \cos^2 \beta - \sin^2 \beta + 1 - 2 \cos \beta + \cos^2 \beta) \\ = \delta_{ij}.$$

This angular displacement is about the $\vec{\beta}$ direction:

$$\alpha_{ij} \beta_j = \beta_i \cos \beta + \beta_i (1 - \cos \beta) = \beta_i.$$

The spur of α_{ij} is

$$\alpha_{ij} = 3 \cos \beta + 1 - \cos \beta \\ = 1 + 2 \cos \beta,$$

so the angle through which the axes are rotated about the $\vec{\beta}$ direction is β . Finally, the infinitesimal transformation is

$$\alpha_{ij} = \delta_{ij} + \epsilon_{ijk} \beta_k$$

$$\chi'_i - \chi_i = \epsilon_{ijk} \chi_j \beta_k \\ = -(\vec{\beta} \times \vec{\chi})_i, \quad (11)$$

and the primed axes are rotated in the right hand sense about the $\vec{\beta}$ direction relative to the unprimed axes. In summary, when $\vec{\beta}$ is real, $\Lambda = \exp(i\frac{1}{2}\vec{\beta} \cdot \vec{\sigma})$ satisfies Eq. (7) and it corresponds to a space rotation with angular displacement vector $\vec{\beta}$. Next the case when $\vec{\beta}$ is pure imaginary may be considered, say

$$\vec{\beta} = i v^{-1} \vec{v} \operatorname{arctanh}(\gamma/c). \quad (12)$$

In this case Eq. (7) becomes

$$\alpha_{\alpha\beta} \sigma_\beta = (\cos \beta/2 + i \vec{\beta} \cdot \vec{\sigma}_\beta \sin \beta/2) \alpha_\alpha (\cos \beta/2 + i \vec{\beta} \cdot \vec{\sigma}_\beta \sin \beta/2),$$

$$\alpha_{4\beta} \sigma_\beta = (\cos^2 \beta/2 - \sin^2 \beta/2) \alpha_4 - 2 \vec{\beta} \cdot \vec{\sigma}_\beta \sin \beta/2 \cos \beta/2$$

$$= \cos \beta \alpha_4 - \sin \beta \vec{\beta} \cdot \vec{\sigma}_\beta,$$

$$\begin{aligned} \alpha_{i\beta} \sigma_\beta &= \cos^2 \beta/2 \alpha_i - \vec{\beta} \cdot \vec{\sigma}_i \vec{\beta} \cdot \vec{\sigma}_\beta \beta^{-2} \sin^2 \beta/2 \\ &\quad + i \beta^{-1} \sin \beta/2 \cos \beta/2 (\alpha_i \vec{\beta} \cdot \vec{\sigma}_\beta + \vec{\beta} \cdot \vec{\sigma}_i \alpha_i) \end{aligned}$$

$$= \alpha_i - \beta_i \vec{\beta} \cdot \vec{\sigma}_\beta^2 (1 - \cos \beta) + \alpha_4 \beta_i / \beta \sin \beta.$$

Eq. (12) implies that the trigonometric functions of β are

$$\sin \beta = \frac{i \gamma/c}{\sqrt{1 - v^2/c^2}},$$

$$\cos \beta = \frac{1}{\sqrt{1 - v^2/c^2}},$$

so the final result for the transformation coefficients is

$$a_{ij} = \delta_{ij} - \frac{v_i v_j}{c^2} \left(1 - \frac{1}{\sqrt{1 - v^2/c^2}} \right) ,$$

$$a_{i4} = \frac{i v_i / c}{\sqrt{1 - v^2/c^2}} , \quad a_{4i} = \frac{-i v_i / c}{\sqrt{1 - v^2/c^2}} , \quad (13)$$

$$a_{44} = \frac{1}{\sqrt{1 - v^2/c^2}} .$$

This is a pure Lorentz transformation with the primed axes moving relative to the unprimed with velocity \vec{v} .¹³ When transformations are compounded the Λ matrices are simply multiplied and the next question is whether products of matrices of the form $\exp(i/2 \beta \cdot \vec{\sigma})$ also are of this form. The answer is yes as can be seen from Hausdorff's¹⁴ theorem which states that

$$e^A e^B = e^{A+B+\frac{1}{2}[A,B]+\frac{1}{12}[A,[A,B]]+\frac{1}{12}[[A,B],B]+\dots} \quad (14)$$

where the higher terms in the series depend only on successively higher order commutators. If this theorem is applied to the product $\exp(i/2 \beta_A \cdot \vec{\sigma}) \exp(i/2 \beta_B \cdot \vec{\sigma})$, since

$$[\frac{1}{2} \beta_A \cdot \vec{\sigma}, \frac{1}{2} \beta_B \cdot \vec{\sigma}] = -\frac{1}{4} \beta_{Ai} \beta_{Bj} [\sigma_i, \sigma_j]$$

$$= -\frac{i}{2} \beta_{Ai} \beta_{Bj} \epsilon_{ijk} \sigma_k$$

$$= -\frac{i}{2} (\beta_A \times \beta_B) \cdot \vec{\sigma} ,$$

all the commutators can in principle be reduced to a term (something) $\vec{\sigma}$ and these can be summed to give the product $\exp(i/2 \beta_{AB} \cdot \vec{\sigma})$. One sees therefore that every Lorentz transformation continuous with the

identity can be generated by $\Lambda = \exp(i\frac{1}{2} \vec{\beta} \cdot \vec{\sigma})$ and that the $\vec{\beta}$ are an acceptable set of parameters for the transformations. One can ask in what sense $\vec{\beta}$ is a vector. The answer is that it is a vector with respect to simultaneous rotations of the primed and unprimed axes. To see this one considers the space rotation described by $\bar{\alpha}_{ij}$, $\bar{\Lambda}$ so that

$$\bar{\alpha}_{ij} \alpha_j = \bar{\Lambda}^H \alpha_i \bar{\Lambda} .$$

For a space rotation $\bar{\Lambda}$ is unitary:

$$\bar{\Lambda}^H = (e^{i\frac{1}{2} \vec{\beta} \cdot \vec{\sigma}})^H = e^{-i\frac{1}{2} \vec{\beta} \cdot \vec{\sigma}} = \bar{\Lambda}^{-1} .$$

Let this rotation be applied to both the primed and unprimed axes, related by

$$\psi' = e^{i\frac{1}{2} \vec{\beta} \cdot \vec{\sigma}} \psi .$$

Then the new wave functions are

$$\bar{\psi}' = \bar{\Lambda} \psi' ,$$

$$\bar{\psi} = \bar{\Lambda} \psi$$

so that

$$\bar{\psi}' = \bar{\Lambda} e^{i\frac{1}{2} \beta_j \alpha_j} \bar{\Lambda}^{-1} \bar{\psi}$$

$$= e^{i\frac{1}{2} \beta_j \bar{\alpha}_{ij} \alpha_i} \bar{\Lambda}^{-1} \bar{\psi}$$

$$= e^{i\frac{1}{2} \beta_i \alpha_i} \bar{\psi}$$

$$= e^{i\frac{1}{2} \bar{\beta}_i \alpha_i} \bar{\psi} ,$$

where

$$\bar{\beta}_i = \bar{a}_{ij} \beta_j$$

as required.

The covariance of the equation with respect to space and time reflections

$$\chi'_i = -\chi_i , \quad t' = t , \quad (15)$$

$$\chi'_i = \chi_i , \quad t' = -t \quad (16)$$

is easily seen by making use of the fact that

$$\sigma_2 \sigma_{\bar{i}} \sigma_2 = -\sigma_i^c . \quad (17)$$

Starting with the equation

$$c \vec{\sigma} \cdot \vec{p}' \psi'(\chi') = i \hbar \frac{\partial}{\partial t'} \psi'(\chi')$$

one substitutes

$$\psi'(\chi') = [\sigma_2 \psi(\chi)]^c \quad (18)$$

in order to obtain

$$c \vec{\sigma} \cdot \vec{p} \psi(\chi) = i \hbar \frac{\partial}{\partial t} \psi(\chi)$$

so that the equation is covariant.

In the theory of spinors, originally discovered by Cartan,¹⁵ a quantity that transforms with respect to the proper Lorentz group according to Eq. (6) is called a spinor of the first rank with lower dotted index and is written a_r so that

$$a'_r(\chi') = \Lambda_{rs} a_s(\chi) .$$

Quantities that transform according to the conjugate of this are given undotted indices:

$$b'_r(x') = \Lambda_{rs}^c b_s(x).$$

Spinors with upper indices are defined by

$$a^{\hat{r}} = \epsilon^{rs} a_{\hat{s}},$$

where $\epsilon^{11} = \epsilon^{22} = 0$ and $\epsilon^{12} = -\epsilon^{21} = 1$, because Λ is uni-modular

$$\begin{aligned} \det \Lambda &= \det e^{i/2 \vec{\beta} \cdot \vec{\sigma}} \\ &= e^{\text{Sp } i/2 \vec{\beta} \cdot \vec{\sigma}} = 1 \end{aligned}$$

so that one forms a scalar (with respect to the proper Lorentz group) by contracting upper with lower indices:

$$\begin{aligned} a'^{\hat{r}} b'_{\hat{r}} &= \epsilon^{rs} a'_{\hat{s}} b'_{\hat{r}} \\ &= \epsilon^{rs} \Lambda_{st} \Lambda_{ru} a_t b_u \\ &= \epsilon^{ut} \det \Lambda a_t b_u \\ &= a^{\hat{u}} b_{\hat{u}}. \end{aligned}$$

A spinor is in a way half way between a scalar and a vector because its transformation coefficients for a space rotation through angle β depend on $\sin \beta/2$ or $\cos \beta/2$. All types of tensors can be formed from spinor products. For example

$$\psi'^{\mu} \sigma_{\mu} \psi' = (\Lambda \psi)^{\mu} \sigma_{\mu} \Lambda \psi$$

$$= \psi^* \wedge^\mu \sigma_\mu \wedge \psi \quad (19)$$

$$= Q_{\mu\nu} \psi^* \sigma_\nu \psi$$

so $\psi^* \sigma_\mu \psi$ is a vector with respect to proper Lorentz transformations. Spinor quantities are of special interest in physics because of the theorem that a quantity with a finite number of components that transforms linearly with respect to proper Lorentz transformations is some rank of spinor.¹⁶ Spinor quantities in the past have been considered only with respect to the proper Lorentz group but it seems appropriate now to consider reflections too and define a spinor to be a quantity that transforms like ψ in the preceding paragraph with respect to the full Lorentz group including reflections.

To find the plane wave solutions of the two-component neutrino equation one substitutes

$$\psi = u e^{i \vec{k} \cdot \vec{r} - Wt} \quad (20)$$

so that the equation reduces to

$$c \vec{\sigma} \cdot \vec{p} u = Wu$$

(the symbol \vec{p} is used for the eigenvalue as well as the operator). Since

$$(c \vec{\sigma} \cdot \vec{p})^2 = c^2 p^2,$$

the only eigenvalues that can arise for W are $\pm cp$. These do give the two solutions which can be written in the form

$$u_\pm = \left(\frac{p_1^2 + p_2^2}{4p^2} \right) \frac{1}{4} \begin{pmatrix} \left(\frac{\pm p + p_3}{p_1 + ip_2} \right)^{1/2} \\ \left(\frac{\mp p + p_3}{p_1 + ip_2} \right)^{-1/2} \end{pmatrix} \quad (21)$$

having the properties

$$c \vec{\sigma} \cdot \vec{p} u_{\pm} = \pm c p u_{\pm} ,$$

$$u_{\pm}^* u_{\pm} = 1 ,$$

$$u_{\pm}^* u_{\mp} = 0 .$$

The assignments for observable quantities, such as energy, momentum, and angular momentum, are made using a hole theory. One expands a solution ψ in terms of the two types of plane waves:

$$\begin{aligned} \psi &= (2\pi\hbar)^{-3/2} \int d^3p \frac{K_+(\vec{p})}{\sqrt{p}} u_+(\vec{p}) e^{i\hbar(\vec{p} \cdot \vec{x} - cpt)} \\ &\quad + (2\pi\hbar)^{-3/2} \int d^3p \frac{K_-(\vec{p})}{\sqrt{p}} u_-(\vec{p}) e^{i\hbar(\vec{p} \cdot \vec{x} + cpt)} \end{aligned} \tag{22}$$

$$\equiv \psi_+ + \psi_- \text{, say.}$$

Then the expected values of the energy, momentum, and angular momentum are

$$\begin{aligned} \mathcal{H} &= \int d^3x \psi_+^* H \psi_+ - \int d^3x \psi_-^* H \psi_- , \\ \vec{p} &= \int d^3x \psi_+^* \vec{p} \psi_+ - \int d^3x \psi_-^* \vec{p} \psi_- , \end{aligned} \tag{23}$$

$$\vec{J} = \int d^3x \psi_+^* (\vec{x} \times \vec{p} + \frac{\hbar}{2} \vec{\sigma}) \psi_+ - \int d^3x \psi_-^* (\vec{x} \times \vec{p} + \frac{\hbar}{2} \vec{\sigma}) \psi_- ,$$

where, since the two-component neutrino is spin 1/2 and so follows Fermi statistics, the wave function is normalized to one particle,

$$\int \psi^* \psi d^3x = 1 .$$

It is clear that this normalization is time-independent and relativistic because, as seen from Eq. (5), $\partial_{K_\alpha} (\psi^\mu \alpha_\mu \psi)$ is zero and, according to Eq. (19), $\psi^\mu \alpha_\mu \psi$ is a 4-vector. Also one can verify that $\psi^\mu \alpha_\mu \psi$ is regular by space reflection and pseudo by time reflection so the normalization is reflection-invariant as well.

For any operator O that commutes with the Hamiltonian

$$\int d^3x \psi_t^\mu O \psi_{\bar{t}} = \pm \frac{1}{2} \int d^3x \psi_{\bar{t}}^\mu \left(\frac{H}{|H|} O - O \frac{H}{|H|} \right) \psi_{\bar{t}} = O. \quad (24)$$

This applies to each of the operators in the equations above so that expected values can be written more briefly as

$$\mathcal{H} = \int d^3x \psi^\mu |H| \psi,$$

$$\vec{P} = \int d^3x \psi^\mu \frac{H}{|H|} \vec{p} \psi, \quad (25)$$

$$\vec{J} = \int d^3x \psi^\mu \frac{H}{|H|} (\vec{x} \times \vec{p} + \hbar/2 \vec{\sigma}) \psi.$$

The operators corresponding to the observable energy, momentum, and angular momentum are $|H|$, $H/|H| \vec{p}$, $H/|H| (\vec{x} \times \vec{p} + \hbar/2 \vec{\sigma})$. The component of the spin in the direction of the momentum is therefore

$$\frac{H}{|H|} \frac{\hbar/2}{\vec{p}/p} \vec{\sigma} \cdot \frac{H}{|H|} \vec{p}/p = \pm \frac{\hbar/2}{p}$$

for the two types of solution. The propagation direction of the two types of wave is $\pm \vec{p}/p$, in the momentum direction.

III. The Photon

Maxwell's theory can be rewritten in a form almost completely parallel to the two-component neutrino theory.¹⁷ One starts with the equations for the free field

$$\epsilon_{jkl} \frac{\partial E_l}{\partial x_k} + \frac{1}{c} \frac{\partial B_j}{\partial t} = O,$$

$$\epsilon_{jkl} \frac{\partial B_l}{\partial x_k} - \frac{1}{c} \frac{\partial E_j}{\partial t} = O, \quad (26)$$

$$\frac{\partial E_i}{\partial x_j} = \frac{\partial B_j}{\partial x_i} = 0$$

and rewrites them in terms of the spinor components. The spinor formulation of the theory was studied by Laporte and Uhlenbeck,¹⁸ the electromagnetic field forms a symmetric spinor of the second rank with components

$$g_{ii} = -2i(\psi_2 + i\psi_1),$$

$$g_{iz} = g_{zi} = -2i(\psi_2 - i\psi_1), \quad (27)$$

$$g_{iz} = g_{zi} = -2\psi_3,$$

where

$$\psi_j = (8\pi c)^{-1/2}(E_j + iB_j).$$

One can just as well work with ψ_1, ψ_2, ψ_3 directly as with g_{ii}, g_{iz}, g_{zi} since they are related by a linear transformation which will only influence the representation of the matrices. Then Eqs. (26) become

$$\epsilon_{jkl} \frac{\partial \psi_k}{\partial x_l} - \frac{i}{c} \frac{\partial \psi_i}{\partial t} = 0, \quad (28)$$

$$\frac{\partial}{\partial x_k} \psi_k = 0 \quad (29)$$

and, in terms of the matrices A_k defined by

$$(A_k)_{jl} = i \epsilon_{jkl}, \quad (30)$$

the curl equations reduce to

$$c \vec{A} \cdot \vec{\nabla} \psi = i \hbar \frac{\partial}{\partial t} \psi. \quad (31)$$

In detail these matrices are

$$\Delta_1 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \quad \Delta_2 = \begin{pmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix}, \quad \Delta_3 = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad (32)$$

and their commutation rules are easily calculated as follows:

$$\begin{aligned} [\Delta_i, \Delta_j]_{kl} &= (\Delta_i)_{km} (\Delta_j)_{ml} - (\Delta_j)_{km} (\Delta_i)_{ml} \\ &= -\epsilon_{kijm} \epsilon_{mjL} + \epsilon_{kjlm} \epsilon_{mil} \\ &= -\delta_{kj} \delta_{il} + \delta_{kl} \delta_{ij} + \delta_{ki} \delta_{jl} - \delta_{ki} \delta_{lj} \\ &= -\epsilon_{ijm} \epsilon_{kml} \\ &= i \epsilon_{ijm} (\Delta_m)_{kl}. \end{aligned}$$

Therefore

$$[\Delta_i, \Delta_j] = i \epsilon_{ijk} \Delta_k \quad (33)$$

and these are angular momentum matrices. It is evident from Eq. (32) that they have eigenvalues 0, ± 1 so they are a representation of spin 1. One sees that the Maxwell equations do take a form similar to that of the two-component neutrino but with the auxiliary condition Eq. (29) still to be taken into account.

The plane wave solutions of Eq. (31) are found by substituting

$$\psi = u e^{i(\vec{p} \cdot \vec{x} - \omega t)} \quad (34)$$

This leads to the matrix eigenvalue problem

$$c \begin{pmatrix} 0 & -ip_3 & ip_2 \\ ip_3 & 0 & -ip_1 \\ -ip_2 & ip_1 & 0 \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ u_3 \end{pmatrix} = W \begin{pmatrix} u_1 \\ u_2 \\ u_3 \end{pmatrix}.$$

The solutions can be written in the form

$$W = \pm cp, 0 ; \quad (35)$$

$$u_{\pm} = \frac{1}{\sqrt{2} p^2(p_1^2 + p_2^2)} \begin{pmatrix} \pm ip p_2 - p_1 p_3 \\ \mp ip p_1 - p_2 p_3 \\ p_1^2 + p_2^2 \end{pmatrix}, \quad u_0 = \begin{pmatrix} p_1 \\ p_2 \\ p_3 \end{pmatrix}. \quad (36)$$

For the plane waves of Eq. (34) the condition $\partial_{x_j} \psi_i = 0$ is the same as $\vec{p} \cdot \vec{u} = 0$. This is satisfied for u_{\pm} but not for u_0 . Therefore one can specify Maxwell's theory by giving the wave equation Eq. (31) and the auxiliary condition that only solutions with $W = \pm cp$ or superpositions of them are to be accepted. One can rewrite these solutions in terms of \vec{E} and \vec{B} ; it is found that the solution propagating in the $\pm \vec{p}$ direction is right/left hand circularly polarized with the propagation direction.

The transformation properties of ψ can be directly deduced from the well-known transformation properties of \vec{E} and \vec{B} . For space rotations ψ is a vector;

$$\psi'_i = Q_{ij} \psi_j ,$$

where Q_{ij} are the orthogonal transformation coefficients. For a pure Lorentz transformation it is known that¹⁹

$$E'_j = \gamma E_j - \frac{v_j v_k}{c^2} (\gamma - 1) E_k + \gamma \epsilon_{jkl} \frac{v_k}{c} B_l ,$$

$$B'_j = \gamma B_j - \frac{v_j v_k}{c^2} (\gamma - 1) B_k - \gamma \epsilon_{jkl} \frac{v_k}{c} E_l ,$$

where

$$\gamma = (1 - \frac{v^2}{c^2})^{-\frac{1}{2}}$$

and v_i is the velocity of the primed system relative to the unprimed. These equations combine to give

$$\psi'_j = \gamma \psi_j - \frac{v_j v_k}{c^2} (\gamma - 1) \psi_k - i \epsilon_{jkl} \gamma \frac{v_k}{c} \psi_l. \quad (37)$$

The transformation coefficients are

$$b_{jk} = \gamma \delta_{jk} - \frac{v_j v_k}{c^2} (\gamma - 1) - i \epsilon_{jlk} \gamma \frac{v_k}{c} \quad (38)$$

and this also is an orthogonal transformation:

$$b_{jk} b_{jm} = \gamma^2 \delta_{km} - \frac{v_k v_m}{c^2} \gamma (\gamma - 1) - i \epsilon_{mjk} \gamma^2 \frac{v_k}{c}$$

$$- \frac{v_k v_m}{c^2} \gamma (\gamma - 1) + \frac{v_k v_m}{c^2} (\gamma - 1)^2 - i \epsilon_{kjm} \gamma^2 \frac{v_k}{c}$$

$$- \epsilon_{jlk} \epsilon_{jnm} \frac{v_k v_n}{c^2} \gamma^2$$

$$= (\gamma^2 - \frac{v^2}{c^2} \gamma^2) \delta_{km} - \frac{v_k v_m}{c^2} (\gamma^2 - 1 - \frac{v^2}{c^2} \gamma^2) = \delta_{km}.$$

Therefore ψ transforms orthogonally for the entire continuous Lorentz group. A three-by-three orthogonal matrix can be written as the exponential of an antisymmetric matrix and the δ_j make a complete set of antisymmetric matrices so it must be possible to write the transformation rule in the form

$$\psi'(\chi') = e^{i \vec{\beta} \cdot \vec{\alpha}} \psi(\chi). \quad (39)$$

This $\vec{\beta}$ is identical with the $\vec{\beta}$ used in the previous section for the two-component neutrino. To see this one proves first that it is a vector in the same sense. With respect to a rotation of axes

$$\bar{x}'_i = \bar{a}_{ij} x_j \quad , \quad \bar{x}_i = \bar{a}_{ij} x_j$$

where

$$\bar{a}_{ij} \bar{a}_{ik} = \delta_{jk} \quad , \quad \det \bar{a} = 1 ,$$

the ψ function here is a vector so

$$\bar{\psi}' = \bar{a} \psi' \quad , \quad \bar{\psi} = \bar{a} \psi .$$

Then one finds that

$$\bar{\psi}' = \bar{a} e^{i \vec{\beta} \cdot \vec{A}} \bar{a}^{-1} \bar{\psi} = e^{i \beta_j \bar{a} \Delta_j \bar{a}^{-1}} \bar{\psi} .$$

However from the definition of the Δ_j , Eq. (30), the following simplification applies:

$$(\bar{a} \Delta_j \bar{a}^{-1})_{kl} = \bar{a}_{km} (\Delta_j)_{mn} (\bar{a}^{-1})_{nl}$$

$$= \bar{a}_{km} i \epsilon_{mjn} \bar{a}_{ln}$$

$$= i \epsilon_{pmn} (\bar{a}_{qj} \bar{a}_{qp}) \bar{a}_{ln} \bar{a}_{km}$$

$$= i (\det \bar{a}) \epsilon_{qjkl} \bar{a}_{qj}$$

$$= (\Delta_q \bar{a}_{qj})_{kl} ,$$

so

$$\bar{\psi}' = e^{i \beta_j \Delta_q \bar{a}_{qj}} \bar{\psi} = e^{i \bar{\beta}_q \Delta_q} \bar{\psi} ,$$

where

$$\bar{\beta}_q = \bar{a}_{qj} \beta_j$$

as required. Next one considers the cases of real and pure imaginary β separately. One can then choose axes so β_1 and β_2 are zero and

$$e^{i\vec{\beta} \cdot \vec{A}} = e^{i\beta A_3} = \sum_{n=0}^{\infty} \frac{\beta^n}{n!} \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}^n$$

$$= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} + \begin{pmatrix} 0 & \beta & 0 \\ -\beta & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} + \frac{1}{2} \begin{pmatrix} -\beta^2 & 0 & 0 \\ 0 & -\beta^2 & 0 \\ 0 & 0 & 0 \end{pmatrix} + \dots$$

$$= \begin{pmatrix} \cos \beta & \sin \beta & 0 \\ -\sin \beta & \cos \beta & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

For real β this is a rotation through angle β about the three-axis in the right-hand sense. Also if one puts here

$$\beta = i \tanh^{-1} \gamma c$$

the matrix becomes

$$e^{i\vec{\beta} \cdot \vec{A}} = \begin{pmatrix} \gamma & i\gamma \gamma c & 0 \\ -i\gamma \gamma c & \gamma & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

and this agrees with Eq. (38) when \vec{U} is specialized to the 3-direction. These arguments show that the $\vec{\beta}$ of Eq. (39) is identical with the $\vec{\beta}$ parameter used for the two-component neutrino for space rotations and for pure Lorentz transformations. Then one can see from Hausdorff's theorem, Eq. (14), that the identification applies always because the calculation of products of transformations depends only on the commutators of the matrices in the exponents and these are the same for the spin one \vec{A} as for the spin one-half $\frac{1}{2}\vec{\sigma}$. One can say then that the transformation

$$\psi'(\chi') = e^{i\vec{\beta} \cdot \vec{\Delta}} \psi(\chi)$$

applies uniformly to the two-component neutrino and the photon as long as one uses the appropriate angular momentum matrices $\vec{\Delta}$. With regard to the space and time reflections

$$\chi'_i = -\chi_i \quad , \quad t' = t \quad ,$$

$$\chi'_i = \chi_i \quad , \quad t' = -t \quad ,$$

it is assumed below that the fields transform according to

$$E'_i(\chi') = E_i(\chi) \quad ,$$

$$B'_i(\chi') = -B_i(\chi) \quad .$$

This agrees with the usual assumption for time-reflection²⁰ and with the space-reflection rule recently proposed by Wigner²¹ and Landau²² to preserve the covariance of the β -decay process with respect to space reflection. For ψ this gives the transformation

$$\psi'(\chi') = [\psi(\chi)]^c \quad . \quad (40)$$

This also agrees with the result for the two-component neutrino, Eq. (18), since for the representation of spin 1 used here

$$\Delta_i = -\Delta_i^c \quad . \quad (41)$$

The next things to consider are the assignments for the energy, momentum, and angular momentum in the field. One writes the general solution of the wave equation and auxiliary condition in the form

$$\begin{aligned} \psi(\chi) = & (2\pi\hbar)^{-\frac{3}{2}} \int d^3 p K_+(\vec{p}) u_+(\vec{p}) e^{i\hbar(\vec{p} \cdot \vec{\chi} - cpt)} \\ & + (2\pi\hbar)^{-\frac{3}{2}} \int d^3 p K_-(\vec{p}) u_-(\vec{p}) e^{i\hbar(\vec{p} \cdot \vec{\chi} + cpt)} \end{aligned} \quad (42)$$

The operators to be considered correspond to the invariance properties of the system. That is, if the transformation

$$\chi'_\mu = \chi'_\mu(x) \quad , \quad \psi' = \psi'(x)$$

carries the equation

$$-c \Delta_k \frac{\partial}{\partial x_k} \psi = \frac{\partial}{\partial t} \psi$$

into the equation

$$-c \Delta_k \frac{\partial}{\partial x_k} \psi' = \frac{\partial}{\partial t} \psi' ,$$

then the operator O defined by

$$\psi'(x) = O \psi(x) \tag{43}$$

gives a conservation equation:

$$\begin{aligned} \frac{\partial}{\partial t} (\psi^H \frac{H}{|H|} O \psi) &= (\frac{\partial \psi}{\partial t})^H \frac{H}{|H|} \psi' + \psi^H \frac{H}{|H|} \frac{\partial \psi'}{\partial t} \\ &= -c (\Delta_k \frac{\partial}{\partial x_k} \psi)^H \frac{H}{|H|} \psi' - c \psi^H \frac{H}{|H|} \Delta_k \frac{\partial}{\partial x_k} \psi' \\ &= -c \frac{\partial}{\partial x_k} \psi^H \Delta_k \frac{H}{|H|} \psi' - c \psi^H \Delta_k \frac{\partial}{\partial x_k} \frac{H}{|H|} \psi' \\ &= -c \frac{\partial}{\partial x_k} (\psi^H \Delta_k \frac{H}{|H|} O \psi). \end{aligned} \tag{44}$$

The density of the conserved quantity is $\psi^H \frac{H}{|H|} O \psi$ and its flux is $c \psi^H \Delta_k (\frac{H}{|H|}) O \psi$. Evidently the theorem will also hold if the $\frac{H}{|H|}$ factor is not included. The transformations which will be considered below are the identity, an infinitesimal space-time displacement, and an infinitesimal space rotation:

$$\chi'_\mu = \chi_\mu , \quad (45a)$$

$$\chi'_\mu = \chi_\mu + \alpha_\mu , \quad (45bc)$$

$$\chi'_j = \chi_j + \epsilon_{jkl} \chi_k ; t' = t , \quad (45d)$$

where α_μ, β_ℓ are smallness parameters (the infinitesimal rotation was given in Eq. (11)). The corresponding wave function transformations are

$$\psi'(x') = \psi(x) , \quad (46abc)$$

$$\psi'(x') = e^{i\beta_\ell A_\ell} \psi(x)$$

$$= \psi(x) + i\beta_\ell A_\ell \psi(x) , \quad (46d)$$

and the Maxwell equations are of course covariant with respect to these transformations. The corresponding operators, defined by Eq. (43), are

$$O_a = 1 , \quad (47a)$$

$$O_{bc} = -i\hbar \frac{\partial}{\partial x_\mu} , \quad (47bc)$$

$$O_d = -i\hbar \epsilon_{lmn} x_m \frac{\partial}{\partial x_n} + \hbar A_\ell . \quad (47d)$$

The calculation of the angular displacement operator, for example, is as follows:

$$\psi'(x) = \psi(x_j - \epsilon_{jkl} x_k \beta_\ell) + i\beta_\ell A_\ell \psi(x)$$

$$= \psi(x) - \frac{\partial \psi}{\partial x_j} \epsilon_{jkl} x_k \beta_l + i \beta_l \Delta_l \psi(x)$$

$$= [1 + i \beta_l (-i \epsilon_{ilk} x_k \frac{\partial}{\partial x_l} + \Delta_l)] \psi(x).$$

The β_l are arbitrary so their coefficients are operators 0 that fit the theorem. The conservation theorem of Eq. (44), applied directly to ψ and these operators, does not yield the classical formulas. However, in terms of the function ϕ defined by

$$\phi = \left| \frac{H}{c} \right|^{-1/2} \psi$$

$$= \frac{1}{(2\pi\hbar)^{3/2}} \int \frac{d^3 p}{\sqrt{p}} K_+ u_+ e^{i\frac{p}{\hbar}(p \cdot \vec{x} - cpt)} \quad (48)$$

$$+ \frac{1}{(2\pi\hbar)^{3/2}} \int \frac{d^3 p}{\sqrt{p}} K_- u_- e^{i\frac{p}{\hbar}(p \cdot \vec{x} + cpt)} ,$$

the following results are obtained:

$$\mathcal{H} = \int d^3 x \frac{E^2 + B^2}{8\pi} = \int d^3 x \phi^* |H| \phi , \quad (49b)$$

$$\vec{P} = \int d^3 x \frac{\vec{E} \times \vec{B}}{4\pi c} = \int d^3 x \phi^* \frac{H}{|H|} \vec{p} \phi , \quad (49c)$$

$$\vec{J} = \int d^3 x \vec{x} \times \frac{\vec{E} \times \vec{B}}{4\pi c} = \int d^3 x \phi^* \frac{H}{|H|} (\vec{x} \times \vec{p} + \hbar \vec{A}) \phi . \quad (49d)$$

It is not immediately clear that the theorem given above, relating the invariance properties to conserved quantities, should apply to the function $\phi(x)$. However, since ϕ is $|H/c|^{-1/2} \psi$, ϕ satisfies the same equations and auxiliary condition as ψ ; so if these are covariant for ψ , they are also for ϕ . The transformation operator for ϕ is found as follows:

$$\phi'(x) = \left| \frac{H}{c} \right|^{-1/2} \psi'(x)$$

$$\begin{aligned}
 &= \left| \frac{H}{c} \right|^{-\frac{1}{2}} O \psi(x) \\
 &= \left| \frac{H}{c} \right|^{-\frac{1}{2}} O \left| \frac{H}{c} \right|^{\frac{1}{2}} \phi(x).
 \end{aligned} \tag{50}$$

For operators O that commute with H this reduces to

$$\phi'(x) = O \phi(x);$$

this applies to the operators in Eq. (47). One obtains the expression on the right in Eq. (49b) from the expectation value of the operator

$\frac{H}{|H|} (-i \hbar \partial/\partial x_4)$, replacing $i \hbar \partial/\partial t$ by H as is permitted when it operates on solutions of the field equations. Proofs of the equalities in Eqs. (49) can be made by expressing the quantities involved separately as integrals in momentum space and comparing the results. Using the expansions of Eqs. (42) and (48), one finds, for example,

$$\int d^3x \frac{(E^2 + B^2)}{8\pi} = \int d^3x c \psi^\mu \psi$$

$$= \int \frac{c}{(2\pi\hbar)^3} d^3x \int d^3p (K_+^c u_+^\mu e^{i\hbar cpt} + K_-^c u_-^\mu e^{-i\hbar cpt}) e^{-i\hbar \vec{p} \cdot \vec{x}} \tag{51}$$

$$\cdot \int d^3q (K_+ u_+ e^{-i\hbar cq t} + K_- u_- e^{i\hbar cq t}) e^{i\hbar \vec{q} \cdot \vec{x}}.$$

The integrals on x are done first:

$$\frac{1}{(2\pi\hbar)^3} \int d^3x e^{i\hbar(\vec{q}-\vec{p}) \cdot \vec{x}} = \delta(\vec{q}-\vec{p}).$$

Then many of the terms drop out because of the orthonormality of the u_{\pm} . The result is

$$\int d^3x \frac{E^2 + B^2}{8\pi} = \int d^3p c (K_+^c K_+ + K_-^c K_-) \tag{52}$$

and a similar calculation gives

$$\int d^3x \phi^\mu H \phi = \int d^3p c (K_+^c K_+ + K_-^c K_-) \tag{53}$$

so Eq. (49b) is verified. The calculation for the momentum begins as follows:

$$\begin{aligned}
 (4\pi c)^{-1} \int d^3x (\vec{E} \times \vec{B})_j &= (4\pi c)^{-1} \int d^3x \epsilon_{jkl} E_k B_l \\
 &= (8\pi i c)^{-1} \int d^3x \epsilon_{jkl} (E_k - i B_k)(E_l + i B_l) \\
 &= \int d^3x \psi_k^* (\Delta_j)_{kl} \psi_l \\
 &= \int d^3x \psi^* \Delta_j \psi .
 \end{aligned} \tag{54}$$

In terms of the momentum integrals this takes the same form as Eq. (51) except with the factor A_j/c . From Eq. (36) it is seen that u_\pm^c is

u_\mp so

$$\begin{aligned}
 u_\pm^* \Delta_j u_\mp &= u_\mp^* \Delta_j u_\mp \\
 &= (u_\mp)_k (i \epsilon_{kjl}) (u_\mp)_l = 0
 \end{aligned}$$

Also it is easily seen that

$$u_\pm^* \Delta_j u_\pm = \pm p_j/p .$$

One of these results implies the other since they are complex conjugates. They can be verified by direct calculation, for example

$$\begin{aligned}
 u_+^* \Delta_3 u_+ &= \frac{1}{2p^2(p_1^2+p_2^2)} (-ip p_2 - p_1 p_3, ip p_1 - p_2 p_3, p_1^2 + p_2^2) \cdot \\
 &\quad \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} ip p_2 - p_1 p_3 \\ -ip p_1 - p_2 p_3 \\ p_1^2 + p_2^2 \end{pmatrix}
 \end{aligned}$$

$$\begin{aligned}
 &= \frac{1}{2p^2(p_1^2 + p_2^2)} \left\{ (-i\bar{p}p_2 - p_1p_3)(-\bar{p}p_1 + i\bar{p}_2p_3) + (i\bar{p}p_1 - p_2p_3)(-\bar{p}p_2 - i\bar{p}_1p_3) \right\} \\
 &= \frac{2\bar{p}p_2^2p_3 + 2\bar{p}p_1^2p_3}{2p^2(p_1^2 + p_2^2)} = p_3/p .
 \end{aligned}$$

The substitution of these results into Eq. (54) yields

$$(4\pi c)^{-1} \int d^3x (\vec{E} \times \vec{B})_j = \int \frac{d^3p}{p} (p_j K_+^c K_+ - p_j K_-^c K_-). \quad (55)$$

Also one verifies directly that

$$\int d^3x \phi^*(H_{||HI|}) p_j \phi = \int \frac{d^3p}{p} (p_j K_+^c K_+ - p_j K_-^c K_-)$$

so Eq. (49c) is justified. The proof of the 3-component of Eq. (49d) can be made in a similar way; one uses the intermediate results

$$\epsilon_{3kl} u_\pm^* \left(\frac{\partial}{\partial p_k} \right) \Delta_l u_\pm = 0 ,$$

$$\epsilon_{3kl} u_\pm^* \left(\frac{\partial}{\partial p_k} \right) \Delta_l u_\mp = 0 ,$$

$$\epsilon_{3kl} u_\pm^* \left(\frac{\partial u_\mp}{\partial p_k} \right) p_l = \pm i p_3/p .$$

It is clear from Eqs. (52) and (55) that $d^3p K_+^c K_+ / p$ are to be interpreted as the number of right or left hand circularly polarized photons in d^3p . The total number of photons is then

$$\begin{aligned}
 N &= \int d^3p (K_+^c K_+ + K_-^c K_-)/p \\
 &= \int d^3x \phi^* \phi .
 \end{aligned} \quad (56)$$

The theorem relating covariances of the equations to conserved quantities is applied without the $H_{||HI|}$ factor to get the integral for the number

of particles but otherwise the H/H_0 factor is always used.

IV. Electromagnetic Multipole Radiation

The fact that Maxwell's equations can be written as a particle type of wave equation permits them to be studied using standard quantum mechanical methods. The multipole radiation problem can be worked out in parallel with the Dirac and Schrödinger radial problems.²³ It turns out that the classical multipole fields are eigenfunctions of the angular momentum and space reflection operators for the electromagnetic field.

The problem is to find functions which satisfy

$$c \vec{A} \cdot \vec{p} \psi = i \hbar \frac{\partial}{\partial t} \psi \quad (57)$$

and the auxiliary condition everywhere except at the origin and which, far from the origin, are outgoing waves. One writes

$$\psi(\vec{x}, t) = w(\vec{x}) e^{-i\omega t/\hbar}$$

so that

$$c \vec{A} \cdot \vec{p} w = Ww \quad (58)$$

and satisfies the auxiliary condition by requiring that W be not zero. The operator

$$\vec{J} = \vec{x} \times \vec{p} + \hbar \vec{A}$$

commutes with the Hamiltonian,

$$[\epsilon_{ijk} x_j p_k + \hbar \Delta_i, c \Delta_i p_i] = \epsilon_{ijk} [x_j, p_k] p_i c \Delta_i + c \hbar [\Delta_i, \Delta_i] p_i$$

$$= i c \hbar \epsilon_{ijk} p_k \Delta_j + i c \hbar \epsilon_{ijk} \Delta_j p_i = 0,$$

so one can solve the problem by simultaneously diagonalizing $J_3, J^2, c \vec{A} \cdot \vec{p}$. The simultaneous eigenfunctions of J_3, J^2 are called the vector spherical harmonics; in the notation of Blatt and Weisskopf²⁴ they are written as $Y_{j,l,m}^M(\theta, \phi)$

and they have the properties

$$\vec{J}^2 Y_{J,l,1}^M = J(J+1) \hbar^2 Y_{J,l,1}^M ,$$

$$\vec{J}_3 Y_{J,l,1}^M = M \hbar Y_{J,l,1}^M ,$$

$$(\vec{x} \times \vec{p}) \cdot (\vec{x} \times \vec{p}) Y_{J,l,1}^M = l(l+1) \hbar^2 Y_{J,l,1}^M ,$$

$$\vec{\Delta} \cdot \vec{\Delta} Y_{J,l,1}^M = 2 Y_{J,l,1}^M ,$$

where J^2 , J_3 on the left are the operators and J on the right and in the subscripts is the quantum number. The operator \vec{J} here is \hbar times Blatt and Weisskopf's operator \vec{J} . The quantum number J may be zero or a positive integer; M may be any integer from $-J$ to $+J$, l is unity when J is zero and otherwise may be $J-1$, J , or $J+1$. One finds the vector spherical harmonics by combining the scalar spherical harmonics and the spin 1 eigenfunctions, using the vector addition coefficients in the usual way.

The vector spherical harmonics give the dependence of the solutions on angles and spin coordinate so one substitutes

$$w = f(r) Y_{J,J+1,1}^M + g(r) Y_{J,J,1}^M + h(r) Y_{J,J-1,1}^M \quad (59)$$

into Eq. (58). Here f , g , h are functions to be determined and g , h are zero when J is zero. The calculations are easily made if one re-writes Eq. (58) in vector form

$$c \hbar \nabla \times \vec{w} = W \vec{w}$$

so as to make use of Hill's²⁵ formulas for the curls of functions of r times the vector spherical harmonics. One of the results is that $J=0$ implies $W=0$ so this possibility is to be discarded. Otherwise the equation reduces to

$$i \left(\frac{J}{2J+1} \right)^{1/2} \left(\frac{df}{dr} + \frac{J+2}{r} f \right) + i \left(\frac{J+1}{2J+1} \right)^{1/2} \left(\frac{dh}{dr} - \frac{J-1}{r} h \right) = \frac{W}{c \hbar} g ,$$

$$i \left(\frac{J}{2J+1} \right)^{1/2} \left(\frac{dg}{dr} - \frac{J}{r} g \right) = \frac{W}{c\hbar} f ,$$

$$i \left(\frac{J+1}{2J+1} \right)^{1/2} \left(\frac{dg}{dr} + \frac{J+1}{r} g \right) = \frac{W}{c\hbar} h .$$

The second and third equations can be used to eliminate f and h from the first so that

$$\frac{d^2g}{dr^2} + \frac{2}{r} \frac{dg}{dr} + \left[\left(\frac{W}{c\hbar} \right)^2 - \frac{J(J+1)}{r^2} \right] g = 0$$

which has the solutions

$$g = i \left(\frac{|W|}{c\hbar} \right)^{1/2} H_{J+1/2}^{(1,2)}(\zeta) ,$$

where

$$\zeta = \left(\frac{|W|}{c\hbar} \right) r$$

and $H^{(1,2)}$ is the first or second Hankel function in the notation of Jahnke and Emde.²⁶ One can now substitute this result back and apply the differentiation formulas for the Bessel functions to determine f and h . For large values of its argument $H^{(1,2)}$ behaves like $\zeta^{-1/2} \exp(\pm i \zeta)$ so to get outgoing waves, the first Hankel function is to be used when W is positive and the second when W is negative. Complete solutions to the problem are then

$$\psi^\pm(J, M, |W|; r, \theta, \varphi, t) = (8\pi c)^{-1/2} (2J+1)^{-1/2} \left(\frac{\pi}{2} \zeta \right)^{1/2} \cdot$$

$$\cdot [\pm J^{1/2} H_{J+1/2}^{(1,2)} Y_{J,J+1,1}^M + i(2J+1)^{1/2} H_{J+1/2}^{(1,2)} Y_{J,J+1}^M] \quad (60)$$

$$\mp (J+1)^{1/2} H_{J-1/2}^{(1,2)} Y_{J,J-1,1}^M] e^{\mp i |W| t / \hbar} ,$$

where the first kind of Hankel function is to be used with the upper signs and the second with the lower. These are eigenfunctions of H , J^2 , J_3 with eigenvalues W , $J(J+1)\hbar^2$, $M\hbar$.

The solutions ψ^\pm are not the conventional electric and magnetic

multipole fields. The conventional fields bear this relation to the ψ^\pm :

$$\psi_{\text{mag}}(J, M, |W|; r, \theta, \varphi, t) = \psi^+ + (-1)^J K P \psi^+, \quad (61)$$

$$\psi_{\text{elec}} = i \psi_{\text{mag}}, \quad (62)$$

where the operators K , P are defined by

$$K \psi(\vec{x}, t) = \psi^c(\vec{x}, t),$$

$$P \psi(\vec{x}, t) = \psi(-\vec{x}, t).$$

Since $\psi'(x') = \psi^c(x)$ for a space reflection, $K P$ is the space reflection operator for the electromagnetic field. It is clear that $K P$ anti-commutes with H , J , $i\hbar \frac{\partial}{\partial t}$ so $K P \psi^\pm$ is again a solution but with opposite signs of W and M . Detailed calculation gives

$$K P \psi^\pm(J, M, |W|) = (-1)^{J+M} \psi^\mp(J, -M, |W|).$$

It is seen then that Eqs. (61) and (62) define solutions of the problem with the properties

$$\left(\frac{H}{|H|}\right) J_3 \psi_{m,e} = M \not{R} \psi_{m,e},$$

$$J^2 \psi_{m,e} = J(J+1) \not{R}^2 \psi_{m,e},$$

$$|H| \psi_{m,e} = |W| \psi_{m,e}, \quad (63)$$

$$K P \psi_{\text{mag}} = (-1)^J \psi_{\text{mag}},$$

$$K P \psi_{\text{elec}} = (-1)^{J+1} \psi_{\text{elec}},$$

where $\psi_{m,e}$ indicates either ψ_{mag} or ψ_{elec} . The proof that these definitions of $\psi_{m,e}$ are identical with the usual definitions is given in reference 23. It is interesting that $\psi_{m,e}$ are eigenfunctions of the angular momentum operator $(\frac{W}{|H|}) J_3$ and the space reflection operator $K P$ but not of the angular displacement operator J_3 or of the Hamiltonian H . Equation (63) corresponds to the well-known fact that, in a pure multipole field, each photon has angular momentum $M\hbar$ about the 3-axis:

$$\begin{aligned} \phi_{m,e}^H \left(\frac{H}{|H|} \right) J_3 \phi_{m,e} &= \left| \frac{W}{C} \right|^{-1} \psi_{m,e}^H \left(\frac{H}{|H|} \right) J_3 \psi_{m,e} \\ &= M\hbar \left| \frac{W}{C} \right|^{-1} \psi_{m,e}^H \psi_{m,e} \\ &= M\hbar \phi_{m,e}^H \phi_{m,e} \end{aligned}$$

V. Massless Particle with Arbitrary Spin

The close parallel between the theories of the two-component neutrino and photon suggests the existence of a general theory of the same type and for any spin $s=1/2, 1, 3/2, \dots$. Such a theory can be worked out in all detail.²⁷

One assumes to begin with the wave equation

$$(c/\Delta) \vec{P} \cdot \vec{\Delta} \phi = i\hbar \frac{\partial}{\partial t} \phi \quad (64)$$

and the auxiliary condition that only solutions with spins parallel or anti-parallel to the momentum are to be accepted. Here $\vec{\Delta}$ are the $2s+1$ by $2s+1$ angular momentum matrices with the factor \hbar not included. The usual representation will be used²⁸ so that the only non-zero elements are

$$(\Delta_1)_{m+1,m} = (\Delta_1)_{m,m+1} = \frac{1}{2} [(\Delta-m)(\Delta+m+1)]^{1/2}, \quad (65)$$

$$(\Delta_2)_{m+1,m} = -(\Delta_2)_{m,m+1} = -\frac{i}{2} [(\Delta-m)(\Delta+m+1)]^{1/2}, \quad (66)$$

$$(\Delta_3)_{mm} = m. \quad (67)$$

Here the subscript m ranges from $-s$ to $+s$ and refers to the row or column which has m on the diagonal in Δ_3 .

The auxiliary condition is to be applied using an expansion on plane waves. If

$$\phi = u e^{i\frac{1}{4}(\vec{p} \cdot \vec{x} - Wt)},$$

then u is to be found from

$$(\gamma_A) \vec{p} \cdot \vec{\Delta} u = W u. \quad (68)$$

By specializing to an axis in the direction of \vec{p} one sees that the auxiliary condition requires

$$W = \pm cp$$

so that the proper free-particle dispersion is obtained. The corresponding solutions of Eq. (68) are

$$(u_{\pm})_m = \left[\frac{p_1^2 + p_2^2}{4p^2} \right]^{\frac{1}{2}\Delta} \left[\frac{(2\Delta)!}{(\Delta+m)!(\Delta-m)!} \right]^{\frac{1}{2}} \left[\frac{\pm p + p_3}{p_1 + ip_2} \right]^m. \quad (69)$$

Here in the first two factors the positive root is to be used. When the spin is half-integral, a uniform assignment of the branches in the last term is to be made; for example, the term can be interpreted as

$$\left[\frac{\pm p + p_3}{p_1 + ip_2} \right]^{\Delta} \left[\frac{\pm p + p_3}{p_1 + ip_2} \right]^{m-\Delta}$$

and some branch chosen for the first factor--there is no ambiguity in the second factor since $s-m$ is always integral. The verification that Eq. (69) does provide the solutions goes as follows:

$$\begin{aligned} (\gamma_A \vec{p} \cdot \vec{\Delta} u_{\pm})_m &= \gamma_A \sum_n (\vec{p} \cdot \vec{\Delta})_{mn} (u_{\pm})_n \\ &= \gamma_A [(p_1 \Delta_1)_{m,m+1} (u_{\pm})_{m+1} + (p_1 \Delta_1)_{m,m-1} (u_{\pm})_{m-1}] \end{aligned}$$

$$+(P_2 A_2)_{m,m+1} (U_{\pm})_{m+1} + (P_2 A_2)_{m,m-1} (U_{\pm})_{m-1}$$

$$+(P_3 A_3)_{mm} (U_{\pm})_m]$$

Here components like $(U_{\pm})_{\Delta+1}$ and $(A_1)_{\Delta,\Delta+1}$ are defined to be given by Eqs. (69) and (65) also; they have been added in combinations that are always zero but permit uniform treatment of all values of m . Then, grouping terms independent of m into a constant D_{\pm} , one finds

$$(\frac{C}{\Delta} \vec{P} \cdot \vec{\Delta} U_{\pm})_m = \frac{C}{\Delta} D_{\pm} \left\{ \frac{p_1 + ip_2}{2} \frac{[(\Delta-m)(\Delta+m+1)]^{1/2}}{[(\Delta+m+1)!(\Delta-m-1)!]^{1/2}} \left[\frac{p_1 + ip_2}{\pm p + p_3} \right]^{\Delta-m-1} \right.$$

$$\left. + \frac{p_1 - ip_2}{2} \frac{[(\Delta-m+1)(\Delta+m)]^{1/2}}{[(\Delta+m-1)!(\Delta-m+1)!]^{1/2}} \left[\frac{p_1 + ip_2}{\pm p + p_3} \right]^{\Delta-m+1} \right\}$$

$$+ P_3 \frac{m}{[(\Delta+m)!(\Delta-m)!]^{1/2}} \left[\frac{p_1 + ip_2}{\pm p + p_3} \right]^{\Delta-m} \Big\}$$

$$= \frac{C}{\Delta} (U_{\pm})_m \left\{ \frac{p_1 + ip_2}{2} (\Delta-m) \pm \frac{p_1 + ip_2}{p_1 + ip_2} \right.$$

$$\left. + \frac{p_1 - ip_2}{2} (\Delta+m) \frac{p_1 + ip_2}{\pm p + p_3} + m P_3 \right\}$$

$$= C \frac{1}{\Delta} (U_{\pm})_m [\frac{1}{2} (\Delta-m)(\pm p + p_3) + \frac{1}{2} (\Delta+m)(\pm p - p_3) + m P_3]$$

$$= \pm c p (U_{\pm})_m .$$

These functions have been chosen normalized:

$$\begin{aligned}
 u_{\pm}^{\mu} u_{\pm} &= \sum_m (u_{\pm})_m^c (u_{\pm})_m \\
 &= \sum_m \left[\frac{p_i^2 + p_2^2}{4p^2} \right]^{\Delta} \frac{(2\Delta)!}{(\Delta+m)!(\Delta-m)!} \left[\frac{(p \pm p_3)^2}{p_i^2 + p_2^2} \right]^m \\
 &= \sum_{m=0}^{2\Delta} \left[\frac{p_i^2 + p_2^2}{4p^2} \right]^{\Delta} \frac{(2\Delta)!}{m!(2\Delta-m)!} \left[\frac{(p \pm p_3)^2}{p_i^2 + p_2^2} \right]^{m-\Delta} \quad (70) \\
 &= \left[\frac{p_i^2 + p_2^2}{4p^2} \right]^{\Delta} \left[\frac{(p \pm p_3)^2}{p_i^2 + p_2^2} \right]^{-\Delta} \left[1 + \frac{(p \pm p_3)^2}{p_i^2 + p_2^2} \right]^{2\Delta} \\
 &= \left[\frac{1}{4p^2} \right]^{\Delta} [p \pm p_3]^{-2\Delta} [p_i^2 + p_2^2 + p^2 \pm 2pp_3 + p_3^2]^{2\Delta} \\
 &= 1.
 \end{aligned}$$

The following additional properties of these solutions are required and can be established in a similar way:

$$u_{\pm}^{\mu} \Delta_i u_{\pm} = \pm i \Delta \frac{p_i}{p}, \quad (71)$$

$$u_{\pm}^{\mu} \Delta_i u_{\mp} = 0,$$

$$u_{\pm}^{\mu} \partial/\partial p_1 u_{\pm} = \pm i \Delta p_2 p_3 / [p(p_i^2 + p_2^2)],$$

$$u_{\pm}^{\mu} \partial/\partial p_2 u_{\pm} = \mp i \Delta p_1 p_3 / [p(p_i^2 + p_2^2)], \quad (72)$$

$$u_{\pm}^{\mu} \partial/\partial p_3 u_{\pm} = 0,$$

$$u_{\pm}^{\mu} \partial/\partial p_i u_{\mp} = 0.$$

The next question to be considered is the covariance of the wave equation and auxiliary condition. The spinor components ψ are defined in terms of the wave function ϕ by the equation

$$\psi = \left| \frac{H}{C} \right|^{A-1/2} \phi. \quad (73)$$

The general solution of the wave equation and auxiliary condition can be written as

$$\begin{aligned} \psi(x) &= \frac{1}{(2\pi\hbar)^{3/2}} \int d^3 p K_+(\vec{p}) p^{A-1} u_+(\vec{p}) e^{i\hbar(\vec{p}\cdot\vec{x}-cpt)} \\ &\quad + \frac{1}{(2\pi\hbar)^{3/2}} \int d^3 p K_-(\vec{p}) p^{A-1} u_-(\vec{p}) e^{i\hbar(\vec{p}\cdot\vec{x}+cpt)} \end{aligned} \quad (74)$$

(the factors of p^{A-1} are included because $K_\pm^c K_\pm$ turn out to be scalars). By extrapolation of the two-component neutrino and photon results, it is assumed that, with respect to a proper Lorentz transformation

$$x'_\alpha = \alpha_{\alpha\beta} x_\beta$$

the spinor components transform according to

$$\psi'(x') = e^{i\vec{p}\cdot\vec{x}} \psi(x). \quad (75)$$

It remains to be shown that this transformation leads to the covariance of the wave equation and auxiliary condition. The covariance follows from the fact that the functions are covariantly defined in the sense that

$$e^{i\vec{p}\cdot\vec{x}} p^A u_\pm(\vec{p}) = e^{i\eta_\pm} p'^A u_\pm(\vec{p}'), \quad (76)$$

where the primed momenta are defined by

$$p'_\alpha = \alpha_{\alpha\beta} p_\beta \quad (77)$$

and the η_\pm are some real functions of \vec{p} . Here p_4 is defined to be $+ip$ when u_+ is considered and $-ip$ when u_- is considered so that the factor $(\pm p + p_3)$ in Eq. (69) can be written as $(p_3 - i p_4)$ and a uniform treatment of u_\pm can be made. To prove Eq. (76) one

considers first pure rotations and begins with the identity

$$e^{-i\vec{\beta} \cdot \vec{\alpha}} \Delta_i e^{i\vec{\beta} \cdot \vec{\alpha}} = \alpha_{ij} \Delta_j . \quad (78)$$

This was shown to be valid for the spin 1/2 matrices in Section II, Eqs. (7), (8), (10). One can see that it is true for all spins by using another theorem of Hausdorff:¹⁴

$$e^{-A} B e^A = B + [B, A] + \frac{1}{2!} [[B, A], A] + \dots . \quad (79)$$

In the evaluation of the right hand side of Eq. (78) from the left, one needs to know only the commutation rules of the matrices and these are the same for all spins. In consequence of Eq. (78), one can see that

$$\begin{aligned} \vec{\alpha} \cdot \vec{p}' e^{i\vec{\beta} \cdot \vec{\alpha}} u_{\pm}(\vec{p}) &= e^{i\vec{\beta} \cdot \vec{\alpha}} p'_i \alpha_{ij} \Delta_j u_{\pm}(\vec{p}) \\ &= e^{i\vec{\beta} \cdot \vec{\alpha}} \vec{p} \cdot \vec{\alpha} u_{\pm}(\vec{p}) \\ &= \pm \Delta p' e^{i\vec{\beta} \cdot \vec{\alpha}} u_{\pm}(\vec{p}). \end{aligned}$$

Therefore $\exp(i\vec{\beta} \cdot \vec{\alpha}) u_{\pm}(\vec{p})$ are proportional to the eigenfunctions of $\vec{\alpha} \cdot \vec{p}'$. They are already normalized,

$$[e^{i\vec{\beta} \cdot \vec{\alpha}} u_{\pm}(\vec{p})]^* [e^{i\vec{\beta} \cdot \vec{\alpha}} u_{\pm}(\vec{p})] = u_{\pm}^*(\vec{p}) u_{\pm}(\vec{p}) = 1 ,$$

so one can conclude that

$$e^{i\vec{\beta} \cdot \vec{\alpha}} u_{\pm}(\vec{p}) = e^{i\eta_{\pm}} u_{\pm}(\vec{p}') ,$$

which verifies Eq. (76) for pure rotations. It is then sufficient to consider only a Lorentz transformation about the 3-axis:

$$x'_1 = x_1 ,$$

$$x'_2 = x_2 ,$$

$$x'_3 = \frac{x_3 - vt}{[1 - v^2/c^2]^{1/2}},$$

$$t' = \frac{(-vx_3/c^2 + t)}{[1 - v^2/c^2]^{1/2}},$$

$$\psi'_m(x') = e^{i\beta m} \psi_m(x).$$

Here β is given by

$$\beta = i \tanh^{-1} v/c$$

$$\text{so } \sin \beta = \frac{i v/c}{[1 - v^2/c^2]^{1/2}},$$

$$\cos \beta = \frac{1}{[1 - v^2/c^2]^{1/2}},$$

and the coordinate transformation can be written as

$$x'_3 = \cos \beta x_3 + \sin \beta x_4,$$

$$x'_4 = -\sin \beta x_3 + \cos \beta x_4,$$

$$x'_3 - i x'_4 = e^{i\beta} (x_3 - i x_4).$$

Then it follows from the definition of the U_{\pm} , Eq. (69), that

$$[e^{i\vec{\beta} \cdot \vec{p}} p^{\alpha} U_{\pm}(\vec{p})]_m = C(p_1, p_2) e^{i\beta m} (p_3 - i p_4)^m$$

$$= C(p'_1, p'_2) (p'_3 - i p'_4)^m$$

$$= p'^{\alpha} U_{\pm}(\vec{p}'),$$

where C is an abbreviation for the function of p_1, p_2 involved. This establishes Eq. (76) for the entire proper Lorentz group. To prove the

covariance one starts with the plane wave expansion in the unprimed system, Eq. (74), and calculates the spinor components in the primed system:

$$\begin{aligned}\psi'(\chi') = & (2\pi\hbar)^{-\frac{3}{2}} e^{i\vec{p} \cdot \vec{\chi}} \int \frac{d^3 p}{p} K_+ p^\mu u_+(\vec{p}) e^{i\frac{\hbar}{k} p_\mu x_\mu} \\ & + (2\pi\hbar)^{-\frac{3}{2}} e^{i\vec{p} \cdot \vec{\chi}} \int \frac{d^3 p}{p} K_- p^\mu u_-(\vec{p}) e^{i\frac{\hbar}{k} p_\mu x_\mu}.\end{aligned}$$

Here one can change the integration variables from p_i to p'_i using the well-known theorem that $\frac{dp}{p} = \frac{dp'}{p'}$:

$$\begin{aligned}\psi'(\chi') = & (2\pi\hbar)^{-\frac{3}{2}} \int \frac{d^3 p'}{p'} K_+ e^{i n_+ p'^\mu} u_+(p') e^{i\frac{\hbar}{k} p'_\mu x'_\mu} \\ & + (2\pi\hbar)^{-\frac{3}{2}} \int \frac{d^3 p'}{p'} K_- e^{i n_- p'^\mu} u_-(p') e^{i\frac{\hbar}{k} p'_\mu x'_\mu}.\end{aligned}$$

This is an expansion on the plane wave solutions in the primed system so it is clear that the wave equation and auxiliary condition are satisfied and the theory is covariant. It is seen also that

$$K'_\pm(\vec{p}') = e^{i n_\pm} K_\pm(\vec{p}) \quad (80)$$

is the rule for finding the expansion coefficients in the primed system. One must keep in mind that, in calculating the correspondence between \vec{p} and \vec{p}' for K_\pm , p_\pm is $\pm ip$.

Reflections can be easily handled by introducing the matrix C defined by

$$C_{m,n} = i^{2m} \delta_{m,-n} \quad . \quad (81)$$

For the first few spins these matrices are

$$C_{\frac{1}{2}} = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}, \quad C_1 = \begin{pmatrix} 0 & 0 & -1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{pmatrix}, \quad C_{\frac{3}{2}} = \begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \end{pmatrix}.$$

It is easily verified that these matrices are Hermitian and unitary and that

$$C \Delta_i = - \Delta_i^c C \quad (82)$$

so that they form a generalization of the charge conjugation matrix to arbitrary spin.

The equations of motion and auxiliary condition are covariant with respect to both space and time reflections,

$$\chi'_i = -\chi_i \quad , \quad \chi'_4 = \chi_4 \quad , \quad (83a)$$

$$\chi'_i = \chi_i \quad , \quad \chi'_4 = -\chi_4 \quad , \quad (83b)$$

if the spinor components are assigned to transform according to

$$\psi'(\chi') = [C \psi(\chi)]^c. \quad (84)$$

To verify this for the space reflection for example one starts with the plane wave expansion for $\psi(\chi)$, Eq. (74), and finds

$$\psi'(\chi') = (2\pi\hbar)^{-3/2} \int d^3 p K_+^c p^{\Delta-1} (Cu_+)^c e^{i\hbar(-\vec{p}\cdot\vec{x} + cpt)}$$

$$+ (2\pi\hbar)^{-3/2} \int d^3 p K_-^c p^{\Delta-1} (Cu_-)^c e^{i\hbar(-\vec{p}\cdot\vec{x} - cpt)}.$$

From the definition of the u_{\pm} , Eq. (69), it follows that

$$(Cu_{\pm})_m^c = \sum_n C_{mn}^c (u_{\pm})_n^c$$

$$= \sum_n (-i)^{2m} \delta_{m,n} \left[\frac{p_1^2 + p_2^2}{4p^2} \right]^{\frac{1}{2}} \left[\frac{(2\Delta)!}{((\Delta+n)!(\Delta-n)!) \Delta!} \right]^{\frac{1}{2}} \left[\frac{\pm p + p_3}{p_1 - i p_2} \right]^{\Delta} \left[\frac{\pm p + p_3}{p_1 + i p_2} \right]^{n-\Delta}$$

$$= (-i)^{2m} \left[\frac{p_1^2 + p_2^2}{4p^2} \right]^{\frac{1}{2}} \left[\frac{(2\Delta)!}{((\Delta+m)!(\Delta-m)!) \Delta!} \right]^{\frac{1}{2}} \left[\frac{\pm p + p_3}{p_1 - i p_2} \right]^{\Delta} \left[\frac{p_1 - i p_2}{\pm p + p_3} \right]^{m+\Delta} \left[\frac{p_1 + i p_2}{p_1 - i p_2} \right]^{m-\Delta}$$

$$\cdot \left[\frac{\mp p + p_3}{\mp p + p_3} \right]^{m+\Delta} \quad (85)$$

$$= (-i)^{2m} \left[\frac{p_1^2 + p_2^2}{4p^2} \right]^{\frac{1}{2}} \left[\frac{(2\Delta)!}{((\Delta+m)!(\Delta-m)!) \Delta!} \right]^{\frac{1}{2}} \left[\frac{\pm p + p_3}{p_1 - i p_2} \right]^{\Delta} \frac{1}{(-1)^{m+\Delta}} \left[\frac{\mp p + p_3}{p_1 + i p_2} \right]^{m+\Delta}$$

$$= \frac{(-i)^{2m}}{(-1)^{m+\alpha}} \left[\frac{\pm p + p_3}{p_1 - ip_2} \right]^\alpha \left[\frac{\mp p + p_3}{p_1 + ip_2} \right]^\alpha (u_\mp)_m \\ = (u_\mp)_m$$

so a plane wave expansion in the primed system also results:

$$\psi'(x') = (2\pi)^{-3/2} \int d^3p K_-^c p^{\alpha-1} u_+ e^{i\frac{p}{\hbar}(\vec{p} \cdot \vec{x}' - cpt')} \\ + (2\pi)^{-3/2} \int d^3p K_+^c p^{\alpha-1} u_- e^{i\frac{p}{\hbar}(\vec{p} \cdot \vec{x}' + cpt')}.$$

The theory is therefore covariant and the relation for transforming the K_\pm is

$$K'_\pm(\vec{p}) = K_\mp^c(\vec{p}). \quad (86a)$$

The time reflection can be treated in a similar way. One must use also the fact that

$$u_\pm(\vec{p}) = u_\mp(-\vec{p})$$

and the result is that the theory is covariant with

$$K'_\pm(\vec{p}) = K_\pm^c(-\vec{p}) \quad (86b)$$

as the transformation rule for the expansion coefficients.

As suggested by the two-component neutrino and photon, the following assignments for number of particles, energy, momentum, and angular momentum are made:

$$N = \int d^3x \phi^\mu \phi, \quad (87)$$

$$\mathcal{H} = \int d^3x \phi^\mu |\mathcal{H}| \phi, \quad (88)$$

$$\vec{P} = \int d^3x \phi^\mu \frac{H}{|\mathcal{H}|} \vec{p} \phi, \quad (89)$$

$$\bar{J} = \int d^3x \phi^* \frac{H}{|H|} (\vec{x} \times \vec{p} + \hbar \vec{\alpha}) \phi , \quad (90)$$

where, according to Eqs. (73) and (74), ϕ is given by

$$\begin{aligned} \phi(x) = & \frac{1}{(2\pi\hbar)^{3/2}} \int d^3p K_+ p^{-1/2} u_+ e^{i\hbar(\vec{p} \cdot \vec{x} - cpt)} \\ & + \frac{1}{(2\pi\hbar)^{3/2}} \int d^3p K_- p^{-1/2} u_- e^{i\hbar(\vec{p} \cdot \vec{x} + cpt)} \end{aligned} \quad (91)$$

It is clear that the arguments of Sec. III, relating invariance properties, operators, and conserved quantities, although they were made in Sec. III only for spin 1, can now be applied for all spins. The four quantities given above are therefore conserved. One can see also that they have transformation properties compatible with these physical assignments by expressing them in terms of the K_{\pm} . For the number of particles one finds

$$\begin{aligned} N = & \int d^3x \frac{1}{(2\pi\hbar)^{3/2}} \int \frac{d^3p}{p^{1/2}} (K_+^c u_+^* e^{i\hbar cpt} + K_-^c u_-^* e^{-i\hbar cpt}) . \\ & e^{-i\hbar \vec{p} \cdot \vec{x}} \int \frac{d^3q}{q^{1/2}} (K_+ u_+ e^{-i\hbar cq t} + K_- u_- e^{i\hbar cq t}) e^{i\hbar \vec{q} \cdot \vec{x}} \end{aligned} \quad (92)$$

$$= \int \frac{d^3p}{p} (K_+^c K_+ + K_-^c K_-) .$$

Then from the transformation properties of K_{\pm} , Eqs. (80) and (86), it is seen that N is a scalar, regular by space and time reflection. Similarly, the energy and momentum can be written as

$$\mathcal{H} = \int \frac{d^3p}{p} (cp K_+^c K_+ + cp K_-^c K_-) , \quad (93)$$

$$\mathbf{P} = \int \frac{d^3p}{p} (\vec{p} K_+^c K_+ - \vec{p} K_-^c K_-) . \quad (94)$$

If one writes \mathbf{p}_4 for $i\hbar/c$, keeping in mind the nonuniform definition of \mathbf{p}_4 , he can combine these equations to read

$$\mathbf{p}_{\mu} = \int \frac{d^3p}{p} (p_{\mu} K_+^c K_+ - p_{\mu} K_-^c K_-) \quad (95)$$

and now the transformation rules for the K_{\pm} show this to be a four-vector. Equations (93) and (94) show it to be regular by space reflection and pseudo by time reflection as required for the energy-momentum. An analogous discussion for the angular momentum is given in reference 27.

VI. Quantization Process

The next question to consider is the quantization of the theory for arbitrary spin.²⁹ The equations of motion for the spinor components are a special case of the general Dirac-Pauli-Fierz theory for which the quantization process was given by Fierz.³⁰ However, the connection between that general theory and the one considered here is complicated for arbitrary spin. Therefore, it is easier below to take advantage of the existence of a wave function and quantize using the coefficients in an expansion on the plane wave solutions. One postulates, therefore, the wave function operator to be

$$\phi(x) = \frac{1}{(2\pi\hbar)^{3/2}} \int d^3p \alpha_+(\vec{p}) u_+(\vec{p}) e^{i\hbar(\vec{p}\cdot\vec{x} - cpt)} \quad (96)$$

$$+ \frac{1}{(2\pi\hbar)^{3/2}} \int d^3p \alpha_-^*(\vec{p}) u_-(\vec{p}) e^{i\hbar(\vec{p}\cdot\vec{x} + cpt)}$$

where α , α^* are the destruction and creation operators fulfilling the commutation or anticommutation rules.³¹

$$[\alpha_{\pm}(\vec{p}), \alpha_{\pm}^*(\vec{q})] = \delta(\vec{p} - \vec{q}) \quad (97)$$

$$[\alpha_{\pm}(\vec{p}), \alpha_{\mp}(\vec{q})] = [\alpha_{\pm}(\vec{p}), \alpha_{\mp}^*(\vec{q})] = [\alpha_{\pm}(\vec{p}), \alpha_{\mp}(\vec{q})]^* = 0$$

As in the unquantized theory the equation

$$\psi(x) = \left| \frac{\hbar}{c} \right|^{1/2} \phi(x)$$

relates the wave function to the spinor components and these operators satisfy the same wave equation and auxiliary condition as in the unquantized theory.

The first question is whether this postulate is made covariantly. Considering first the proper transformations, one can assign the same transformation rule as in the unquantized theory:

$$\psi'(x') = e^{i\vec{\beta}\cdot\vec{\sigma}} \psi(x)$$

Then since α_+ corresponds to $p^{-\frac{1}{2}} K_+$ and α_-^* to $p^{-\frac{1}{2}} K_-$, the covariance of the wave equation and auxiliary condition follows if the operators transform according to

$$p'^{\frac{1}{2}} \alpha'_\pm(\vec{p}') = e^{\pm i \eta_\pm} p^{\frac{1}{2}} \alpha_\pm(\vec{p}) \quad (98)$$

with p_4 defined nonuniformly as $\pm ip$. Also this equation, together with the property of the delta function,

$$p' \delta(\vec{p}' - \vec{q}') = p \delta(\vec{p} - \vec{q}), \quad (99)$$

assures the covariance of all the commutation rules.

With regard to the space and time reflections

$$\chi'_i = -\chi_i, \quad t' = t, \quad (100a)$$

$$\chi'_i = \chi_i, \quad t' = -t, \quad (100b)$$

the correct transformation rules are found to be

$$\psi'(\chi') = [C \psi(\chi)]^*, \quad (101a)$$

$$\psi'(\chi') = [C \psi(\chi)]^c \quad (101b)$$

with the operator relations

$$\alpha'_\pm(\vec{p}) = \alpha_\mp(\vec{p}), \quad (102a)$$

$$\alpha'_\pm(\vec{p}) = \alpha_\pm^c(-\vec{p}). \quad (102b)$$

The proof of the covariance of the postulated form of the spinor components, for the space reflection for example, is as follows:

$$\psi'(\chi') = \frac{C^c}{(2\pi)^{\frac{3}{2}}} \int d^3 p p^{\frac{1}{2}} [\alpha_+ u_+ e^{i\frac{p}{\hbar}(\vec{p} \cdot \vec{x} - cpt)} + \alpha_-^* u_- e^{i\frac{p}{\hbar}(\vec{p} \cdot \vec{x} + cpt)}]^*$$

$$\begin{aligned}
 &= \frac{1}{(2\pi\hbar)^{\frac{3}{2}}} \int d^3p \ p^{4-\frac{1}{2}} [a_+^*(C_{u+})^c e^{-i\frac{p}{\hbar}\vec{x} - cpt} + a_-^*(C_{u-})^c e^{-i\frac{p}{\hbar}\vec{x} + cpt}] \\
 &= \frac{1}{(2\pi\hbar)^{\frac{3}{2}}} \int d^3p \ p^{4-\frac{1}{2}} [a'_+ u_+ e^{i\frac{p}{\hbar}\vec{x}' - cpt'} + a'_- u_- e^{i\frac{p}{\hbar}\vec{x}' + cpt'}].
 \end{aligned}$$

The commutation rules are obviously covariant by Eq. (102a) also. A similar proof applies for the time reflection. For later purposes it is convenient to choose a representation in which a_{\pm} is real, except perhaps for a phase factor as introduced by Eq. (98). This has the effect that $(a_{\pm}^* a_{\pm})^c$ can be replaced by $a_{\pm}^* a_{\pm}$ in considering time reflections.

The operator assignments for the number of particles, the energy, and the momentum are:

$$N = \int d^3p (a_+^* a_+ + a_-^* a_-), \quad (103)$$

$$\mathcal{H} = \int d^3p (cp a_+^* a_+ + cp a_-^* a_-), \quad (104)$$

$$\vec{P} = \int d^3p (\vec{p} a_+^* a_+ - \vec{p} a_-^* a_-). \quad (105)$$

One finds these q-number energy and momentum assignments by summing the number of particles operator $a_{\pm}^* a_{\pm}$ times the eigenvalue of the c-number energy operator $|H|$ and momentum operator $H/|H| \vec{p}$. The facts that N is a scalar and $(p, i\mathcal{H}/c)$ a four-vector pseudo by time reflection follow directly from the transformation rules for the a_{\pm} .

All the discussion above applies uniformly to both Bose-Einstein and Fermi-Dirac statistics. A non-uniformity comes in when N , \mathcal{H} , \vec{P} are expressed in terms of the wave function. One finds

$$N = \int d^3x \phi^* \phi,$$

$$\mathcal{H} = \int d^3x \phi^* (H/|H|) H \phi,$$

$$\vec{P} = \int d^3x \phi^* (H/|H|) \vec{p} \phi$$

for Bose statistics (infinite constants are disregarded and a sum on the

wave function component indices is understood) and, on the other hand,

$$N = \int d^3x \phi^*(H/H) \phi ,$$

$$\mathcal{H} = \int d^3x \phi^* H \phi ,$$

$$\vec{P} = \int d^3x \phi^* \vec{p} \phi$$

for Fermi statistics. In contrast to the c-number theory, the quantized energy operator is also the Hamiltonian for this system since

$$[\phi, \mathcal{H}]_- = i\hbar \frac{\partial \phi}{\partial t}$$

as is easily verified.

In this theory one finds a direct connection between the spin and the statistics of the particles by considering the commutation rules between the spinor components at different space points. These commutation rules are

$$[\psi_m(\vec{x}, t), \psi_n^*(\vec{x}', t)]_{\pm} = \frac{1}{(2\pi\hbar)^3} \int d^3p p^{4-\frac{1}{2}} (a_+(\psi_m)_m e^{i\hbar(\vec{p}\cdot\vec{x}-cpt)} + a_-^*(\psi_m)_m e^{i\hbar(\vec{p}\cdot\vec{x}'+cpt)}) ,$$

$$= \frac{1}{(2\pi\hbar)^3} \int d^3q q^{4-\frac{1}{2}} (a_+^*(\psi_n)_n e^{-i\hbar(\vec{q}\cdot\vec{x}'-cq't)} + a_-(\psi_n)_n e^{-i\hbar(\vec{q}\cdot\vec{x}'+cq't)}) , \quad (106)$$

$$= \frac{1}{(2\pi\hbar)^3} \int d^3p p^{2\alpha-1} [(a_+(\psi_m)_m (\psi_n)_n^c \pm (a_-(\psi_m)_m (\psi_n)_n^c)] e^{i\hbar(p\cdot(\vec{x}-\vec{x}'))} ,$$

$$[\psi_m(\vec{x}, t), \psi_n(\vec{x}', t)]_{\pm} = 0 . \quad (107)$$

Incidentally it is easy at this point to see how the quantization rules for the two-component neutrino and photon come out of this theory. For the two-component neutrino one specializes to spin 1/2 and Fermi statistics. Then ψ_{\pm} form a complete set so $(\psi_+)_m (\psi_+)_n^c + (\psi_-)_m (\psi_-)_n^c$ is simply δ_{mn} and

$$[\psi_m(\vec{x}, t), \psi_n^*(\vec{x}', t)]_+ = \delta_{mn} \delta(\vec{x} - \vec{x}') \quad (108)$$

For the photon one specializes to spin 1 and Bose statistics to find

$$\begin{aligned}
 [\psi_m(\vec{x}, t), \psi_n^*(\vec{x}', t)]_- &= \frac{1}{(2\pi c)^3} \int d^3 p \, p \cdot [(\psi_+)_m (\psi_+)_n^c - (\psi_-)_m (\psi_-)_n^c] e^{i\vec{p} \cdot (\vec{x} - \vec{x}')} \\
 &= \frac{1}{c} \sum_k \frac{H_{mn}(\vec{x})}{(2\pi c)^3} \int d^3 p \left[(\psi_+)_k (\psi_+)_n^c + (\psi_0)_k (\psi_0)_n^c + (\psi_-)_k (\psi_-)_n^c \right] \cdot \\
 &\quad \exp i/\hbar (\vec{p} \cdot (\vec{x} - \vec{x}')) \\
 &= \frac{1}{c} H_{mn}(\vec{x}) \delta(\vec{x} - \vec{x}') ,
 \end{aligned}$$

where the factor of $H(\vec{x})$ permitted the zero-eigenvalue function ψ_0 to be included also in order to again make a complete set. In the representation of Section III this reads

$$[\psi_m(\vec{x}, t), \psi_n^*(\vec{x}', t)]_- = \hbar \epsilon_{mnk} \frac{\partial}{\partial x'_k} \delta(\vec{x} - \vec{x}'). \quad (109)$$

One can decompose the operator ψ_j ; in terms of two Hermitian operators E_j , B_j according to

$$\begin{aligned}
 E_j &= \frac{1}{2}(8\pi c)^{1/2} (\psi_j + \psi_j^*) , \\
 \psi_j &= \frac{E_j + iB_j}{\sqrt{8\pi c}} , \\
 B_j &= -\frac{i}{2}(8\pi c)^{1/2} (\psi_j - \psi_j^*).
 \end{aligned}$$

Then it is easily verified that \vec{E} , \vec{B} fulfill Maxwell's equations and so are to be identified with the operators of the electromagnetic field. From Eqs. (107) and (109) their commutation rules are found to be

$$[E_i(\vec{x}, t), E_j(\vec{x}', t)]_- = [B_i(\vec{x}, t), B_j(\vec{x}', t)]_- = 0 ,$$

$$[E_i(\vec{x}, t), B_j(\vec{x}', t)]_- = 4\pi i c \hbar \epsilon_{ijk} \frac{\partial}{\partial x'_k} \delta(\vec{x} - \vec{x}') ,$$

in agreement with the usual treatment.³²

To continue the general discussion, one next substitutes for ψ_\pm from Eq. (69) into Eq. (106):

$$\begin{aligned}
 [\psi_m(\vec{x}, t), \psi_n^*(\vec{x}', t)]_{\pm} &= \frac{1}{(2\pi\hbar)^3} \int d^3 p \, p^{2\Delta-1} \left[\frac{p_1^2 + p_2^2}{4p^2} \right]^{\Delta} \left[\frac{(2\Delta)! (2\Delta)!}{(\Delta+m)!(\Delta-m)!(\Delta+n)!(\Delta-n)!} \right]^{1/2} \\
 &\cdot \left(\frac{1}{|p_1^2 + p_2^2|^{\Delta}} \left[(p+p_3)^{2\Delta} \left(\frac{p+p_3}{p_1 + ip_2} \right)^{m-\Delta} \left(\frac{p+p_3}{p_1 - ip_2} \right)^{n-\Delta} \right]_{\pm} \right. \\
 &\quad \left. (p-p_3)^{2\Delta} \left(\frac{-p+p_3}{p_1 + ip_2} \right)^{m-\Delta} \left(\frac{-p+p_3}{p_1 - ip_2} \right)^{n-\Delta} \right] e^{i/\hbar \vec{p} \cdot (\vec{x} - \vec{x}')} \\
 &= \frac{1}{(2\pi\hbar)^3} \int \frac{d^3 p}{p^{2\Delta}} \left[\frac{(2\Delta)! (2\Delta)!}{(\Delta+m)!(\Delta-m)!(\Delta+n)!(\Delta-n)!} \right]^{1/2} (p_1 + ip_2)^{\Delta-m} \\
 &\quad (p_1 - ip_2)^{\Delta-n} \left[(p+p_3)^{m+n} \pm (-1)^{2\Delta} (-p+p_3)^{m+n} \right] e^{i/\hbar \vec{p} \cdot (\vec{x} - \vec{x}')}.
 \end{aligned}$$

To study this expression qualitatively one can choose 3-axis in the $\vec{x} - \vec{x}'$ direction and introduce polar coordinates according to

$$p_1 = p \sin \theta \cos \varphi \quad , \quad p_2 = p \sin \theta \sin \varphi ,$$

$$p_3 = p \cos \theta ,$$

$$\frac{1}{\hbar} \vec{p} \cdot (\vec{x} - \vec{x}') = p \alpha \cos \vartheta ,$$

$$p_1 + ip_2 = p e^{i\varphi} \sin \theta$$

where α is an abbreviation for $i\vec{x} - \vec{x}'/\hbar$. The commutator becomes

$$\begin{aligned}
 [\psi_m(\vec{x}, t), \psi_n^*(\vec{x}', t)]_{\pm} &= \frac{1}{(2\pi\hbar)^3} \int p \sin \theta \, dp \, d\theta \, d\varphi \left[\frac{(2\Delta)! (2\Delta)!}{(\Delta+m)!(\Delta-m)!(\Delta+n)!(\Delta-n)!} \right]^{1/2} \\
 &\cdot e^{i(\Delta-m)\varphi - i(\Delta-n)\varphi} p^{2\Delta-m-n} (\sin \theta)^{2\Delta-m-n} p^{m+n}.
 \end{aligned}$$

$$\cdot [(1+\cos\theta)^{m+n} \pm (-1)^{2\Delta} (1-\cos\theta)^{m+n}] e^{ip\alpha \cos\theta}$$

$$= \frac{2\pi \delta_{mn}}{(2\pi\hbar)^3} \iint \frac{\sin\vartheta d\vartheta dp (2\Delta)!}{2^{2\Delta} (\Delta+m)! (\Delta-m)!} p^{2\Delta+1} (\sin^2\vartheta)^{\Delta-m} .$$

$$\cdot [(1+\cos\theta)^{2m} \pm (1-\cos\theta)^{2m}] e^{ip\alpha \cos\theta}$$

$$= \delta_{mn} \sum_k c_k I(2\Delta+1, k)$$

$$\text{where } I(2\Delta+1, k) = \iint \sin\vartheta d\vartheta dp p^{2\Delta+1} \cos^k \vartheta e^{ip\alpha \cos\theta} .$$

Here the last step is to be carried out by simplifying into powers of $\cos\theta$. It is clear that for Fermi statistics only even powers k arise and for Bose statistics only odd powers. Also $2s + 1$ is even for half-integral spin and odd for integral spin. When k and $2s + 1$ are both even or both odd,

$$I(2\Delta+1, k) = \frac{1}{i^k} \frac{d^k}{d\alpha^k} \iint \sin\vartheta d\vartheta dp p^{2\Delta+1-k} e^{ip\alpha \cos\theta}$$

$$= \frac{1}{i^k} \frac{d^k}{d\alpha^k} \int dp \left. \frac{e^{ip\alpha \cos\theta}}{-ip\alpha} \right|_0^\pi p^{2\Delta+1-k}$$

$$= \frac{1}{i^k} \frac{d^k}{d\alpha^k} \cdot \frac{2}{\alpha} \int dp p^{2\Delta-k} \sin p\alpha$$

$$= \frac{1}{i^k} \frac{d^k}{d\alpha^k} \cdot \frac{2}{\alpha} \frac{d^{2\Delta-k}}{d\alpha^{2\Delta-k}} (-1)^{\frac{1}{2}(2\Delta+1-k)} \int \cos p\alpha dp$$

$$= (-1)^{\frac{1}{2}(2\Delta+1-k)} \frac{2\pi}{i^k} \frac{d^k}{d\alpha^k} \cdot \frac{1}{\alpha} \frac{d^{2\Delta-k}}{d\alpha^{2\Delta-k}} \delta(\alpha) .$$

For half-integer Fermions and integer Bosons only this type of term arises in the commutator so one concludes

$$[\psi_m(\vec{x}, t), \psi_n^*(\vec{x}', t)]_\pm = 0 \quad \text{if } \vec{x} \neq \vec{x}'$$

for this type of particle. On the other hand, when one of $2s + 1$, k is even and the other is odd, one finds

$$I(2s+1, k) = (-1)^{\frac{1}{2}(2s-k)} \frac{2}{ik} \frac{d^k}{dx^k} \frac{1}{\alpha} \frac{d^{2s-k}}{dx^{2s-k}} \frac{P(\alpha)}{\alpha}$$

where Heitler's notation for the P function is used.³³ Therefore, for integer Fermions and half-integer Bosons the commutator is not zero when $\vec{x} \neq \vec{x}'$. In a physically meaningful theory one expects such a commutator to be zero because it follows then that any local interaction which is linear in the spinor components of the interacting particles,

$$H_{int.} = \psi_A \psi_B \dots + \psi_A^* \psi_B^* \dots ,$$

and which involves an even number of Fermions commutes with itself when evaluated for two space-like events. If a system did not have this property an interaction at one point would interfere with an interaction at a different point so there would be an instantaneous communication between the points. This demonstration of the connection between spin and statistics is equivalent to Pauli's³⁴ for Bosons but his argument for Fermions does not apply here since the energy is positive definite for all spins.

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STRANGE PARTICLES AND THEIR INTERACTIONS*

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The purpose of these few lectures is to present some typical facts and ideas from the field of elementary particles--especially strange particles and their strong and weak interactions. This short survey is very sketchy and not at all complete; many important facts have been omitted. The intention is only to show in a simplified way some of the theoretical methods and approaches used in this interesting field.

The first few lectures are devoted to a discussion of the strong interaction occurring in production and scattering processes of strange particles. One finds here a striking similarity to the pion-nucleon interactions; in particular it will be seen that the concept of isotopic spin conservation can be generalized and gives rise to the conservation of strangeness. As a general reference for these strong interactions, the review article by R. H. Dalitz in Reports on Progress in Physics, Vol. XX, 163 (1957) should be consulted.

The second part of these lectures deals with a discussion of the weak interactions. Weak interactions are--with the exception of a few radiative decays--responsible for the decay processes of elementary particles into lighter ones. Because in scattering processes the strong interactions usually mask the weak, the decay processes are in fact almost exclusively the means of studying weak interactions. As a general reference the excellent review article by Gell-Mann and Rosenfeld in Annual Review of Nuclear Science, Vol. 7, 407 (1957) should be consulted. Since this article appeared, the experimental and theoretical situation, especially regarding β decay, has further improved, and some of the new developments are therefore included in these lectures.

I. Elementary Particle Properties

The existence of strange particles was first established by Butler and Rochester in 1947; intensive further research in cosmic ray physics led in a relatively short time to the discovery of most of the presently known particles. Since the development of the high energy machines at Berkeley and Brookhaven, laboratory production of these particles has been made possible, and a tremendous amount of data has been accumulated. In Table I are listed the spin, mass, and lifetimes of the presently known particles. By way of example, a method for measuring mass and

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one for measuring lifetime follow.

Table I
Spin, mass, and lifetime of elementary particles*

Particle	Spin	Mass (Mev)	Mean life (sec)
Photon γ		0	stable
$\nu, \bar{\nu}$	1/2	0	stable
Leptons e^-, e^+	1/2	0.510976	stable
μ^-, μ^+	1/2	105.70 ± 0.06	$(2.22 \pm 0.02) \times 10^{-6}$
π^\pm	0	139.63 ± 0.06	$(2.56 \pm 0.05) \times 10^{-8}$
Mesons π^0	0	135.04 ± 0.16	$0 < \tau < 0.4 \times 10^{-15}$
K^+, \bar{K}^+	0	494.0 ± 0.20	$(1.224 \pm 0.013) \times 10^{-8}$
K^0, \bar{K}^0	0	493 ± 5	$K_1^0 (0.99 \pm 0.08) \times 10^{-10}$ $K_2^0 (9.0 \pm 3.5) \times 10^{-8}$
p, \bar{p}	1/2	938.21	stable
n, \bar{n}	1/2	939.51	$(1.04 \pm 0.13) \times 10^3$
Baryons $\Lambda, \bar{\Lambda}$	1/2	1115.2 ± 0.13	$(2.60 \pm 0.16) \times 10^{-10}$
$\Sigma^+, \bar{\Sigma}^+$	1/2	1189.3 ± 0.35	$(0.85 \pm .10) \times 10^{-10}$
$\Sigma^-, \bar{\Sigma}^-$	1/2	1196.4 ± 0.5	$(1.72 \pm 0.17) \times 10^{-10}$
$\Sigma^0, \bar{\Sigma}^0$	1/2	1188.8 ± 2	$< 0.1 \times 10^{-10}$
$\Xi^-, \bar{\Xi}^-$?	1321 ± 3.5	$(4.6 - 200) \times 10^{-10}$
$\Xi^0, \bar{\Xi}^0$?	?	?

One method of measuring the mass of K particles is to simultaneously measure their momentum and their range in an emulsion.¹ The K particles may be produced by, say, bombarding a tantalum target with the bevatron beam. The beam containing the K particles is then focussed by quadrupole lenses, passed through a sector magnet for momentum analysis, and stopped in an emulsion stack. The region where the K particles are stopped is fairly well defined; the momentum and range can thus be determined.

A method of measuring lifetimes is shown in Fig. 1.² Suppose we have a beam of K^+ particles, and look for the known decay $K_{\mu 2} \rightarrow \mu^+ + \nu$.

* Based upon Table I, page 411, Annual Reviews of Nuclear Science, 1957, by Gell-Mann and Rosenfeld.

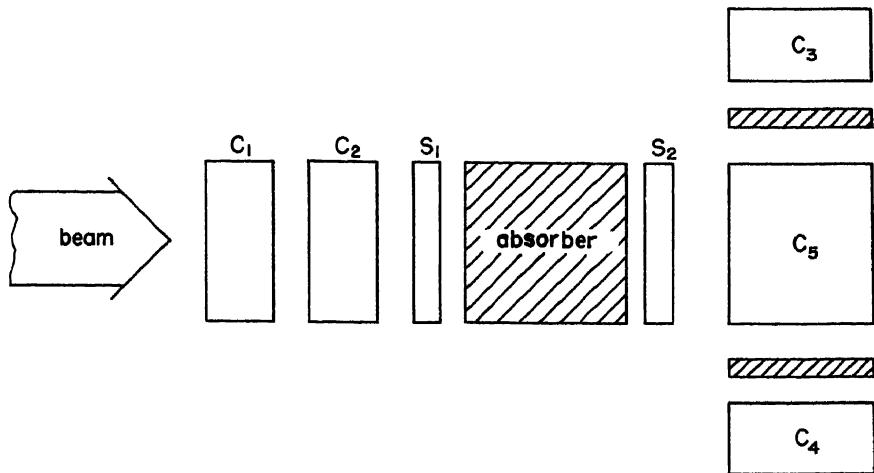


Fig. 1 Apparatus for measuring $K_{\mu 2}^+$ lifetime (see text).

We first analyze the momentum of the beam, and then let it pass through the counting arrangement. C_1 , C_2 , C_3 , and C_4 are Cerenkov counters: C_1 is biassed to count in the region of v_K , the velocity of the K particle, and C_2 is biassed to count in a higher velocity region, corresponding to the velocity of the pions in the beam. S_1 and S_2 are scintillation counters; the absorber between them is intended to slow down the K^+ particle. The K^+ are then stopped in the Cerenkov counter C_5 ; the mesons from the decay are observed by the counters C_3 and C_4 . C_1 and C_2 are used in anticoincidence, and C_1 , C_5 in coincidence with S_1 and S_2 . This insures that a K^+ particle has come into the stopping counter. This system is put in delayed coincidence with C_3 or C_4 ; the amount of delay then measures the lifetime of the particle.

Between the elementary particles listed there are four basic types of interaction, classified by their strength. A measure of this strength is the magnitude of a dimensionless constant, analogous to the well-known fine structure constant in electromagnetic interactions. The four types are:

(a) Strong interactions: the dimensionless constant is in this case

$$\frac{g^2}{4\pi\hbar c} \approx 15$$

where g is the Yukawa coupling constant.

- (b) Electromagnetic interactions: the constant here is

$$\frac{e^2}{4\pi\hbar c} = \frac{1}{137},$$

e being the elementary charge.

- (c) Weak interactions: a typical weak interaction is the β decay. The coupling constant in this process is

$$C_\beta \approx 1.41 \times 10^{-49} \text{ erg-cm}^3.$$

A logical choice for a dimensionless constant involves the Compton wavelength for the π meson, and is

$$C_\beta^2 (\hbar c)^{-2} (\hbar/m_\pi c)^{-4} \approx 5 \times 10^{-14}$$

- (d) Gravitational interaction: the characteristic constant here is

$$\frac{K m_p^2}{\hbar c} \approx 2 \times 10^{-39},$$

K being the gravitational constant, m_p the proton mass.

We shall now discuss some further properties describing the particles and the various interactions, namely the conservation laws. There exist two kinds of conservation laws: those that are strictly valid, and those that are only approximately valid, that is, that hold only if some of the interactions can be neglected. It is these latter that we are most interested in and which we shall discuss in some detail.

First, however, briefly consider the strict conservation laws. It is well known that to a conservation law one can, in a mathematical way, relate an invariance principle. Where this is useful, we shall mention the corresponding invariance.

Strict conservation laws and invariances

Conservation of charge. This conservation law is well established experimentally. The corresponding invariance principle is the gauge invariance.

Conservation of baryon number. This law is also on very firm experimental ground. Baryons are the heavy fermions listed in the third section of Table I, and include, therefore, nucleons and hyperons. The law states that the number of baryons minus the number of antibaryons is a constant.

In principle one can associate an invariance principle with this law, and a number of such principles are to be found in the literature. None of these have been generally accepted, however, so we shall omit them.

A similar law, though less firmly established, seems to hold also for the leptons, or light fermions. It states similarly that the number of

leptons minus the number of antileptons is a constant.

Conservation of energy and momentum. The invariance principle here is translation invariance of physical laws in space and time.

Invariance under proper Lorentz transformation. A special consequence of this invariance is the conservation of angular momentum.

CPT invariance. The CPT invariance follows essentially from the requirements of hermiticity and causality imposed on the Lagrangian. The operators C, P, and T are respectively the charge conjugation, parity, and time reversal operators. The operator P performs a reflection of space coordinates; the operator T gives a reversal of the ordering of events in time; and the operator C changes particles into their corresponding antiparticles.

The CPT theorem states that while each of the operators C, P, and T does not necessarily commute with the Hamiltonian, the product does, and hence guarantees that to each particle there necessarily exists an antiparticle with reversed spin, momentum and space coordinates. The antiparticle may or may not be identical with the particle; the invariance implies that particle and antiparticle have equal masses and, at least to first order, equal lifetimes. For details on this theorem, see reference 3.

CP invariance, and, from CPT, T invariance. From present data on weak interactions it is strongly suggested that a separate invariance under the operation CP, and therefore also T, holds.⁴

The CP invariance gives rise to the strict conservation of a quantum number, the eigenvalue of the CP operator. The S matrix carrying the system from its initial state to its final state must therefore commute with CP. This quantum number is not, however, as powerful in this respect as the parity quantum number in a system conserving parity is, because the eigenstates of the CP operator necessarily describe only neutral systems.

One would think T invariance would also give rise to the conservation of a quantum number, but this is not true; T invariance implies a connection of the phases of the S-matrix elements. To see this, consider the relation

$$U_B = S U_A$$

with S connecting the final state U_B with the initial state U_A . Invariance under T means that the final state (with reversed momenta, etc.) should lead back into the initial state,

$$T U_A = S T U_B$$

Therefore

$$TS = S^{-1}T$$

and it follows that

$$TS = S^* T$$

connecting the hermitian conjugate of S with the unconjugated matrix.

Approximate conservation laws and invariances

Let us now discuss the approximate conservation laws and invariances. These are of particular interest because they characterize the interaction for which they hold.

The separate invariance under C and P. This invariance seems to hold strictly in strong and electromagnetic interactions, but is violated in the weak interactions.

Isotopic spin conservation. The third component of the isotopic spin vector is conserved for strong and electromagnetic interactions. It will be seen that this fact can be expressed as the conservation of strangeness. The square of the total isotopic spin is conserved only in strong interactions.

Decays by weak interactions into strongly interacting particles (like the Λ decay into nucleon and pion), where all particles involved have definite isotopic spin values, show that there is no conservation of isotopic spin in weak interactions. In other weak decays one therefore does not even assign isotopic spin values to the particles involved (lepton, γ quanta) since it would lead to no consequences.

$\frac{1}{2}\psi$, or chirality invariance. Weak interactions seem to show an invariance under the operation $\psi \rightarrow \frac{1}{2}\psi$ for any spinor particle described by ψ .⁵

This invariance holds also for electromagnetic interactions, but is not true for strong interactions. Only the interaction part of the Hamiltonian has this invariance; it obviously does not hold for the mass terms of the free particle part. This is analogous to the isotopic spin symmetry, which holds for the pion-nucleon interaction but not for the mass terms, if the difference in mass between charged and neutral particles is taken into account.

We shall discuss some of these approximate conservation laws in more detail later. Table II summarizes the various laws and the interactions in which they apply.

II. Strong Interactions

The strangeness quantum number

The strangeness of the new particles lies in the fact that, while they interact strongly with nucleons and with each other (their production cross section is of the order of a few millibarns), and decay again into strongly interacting particles, their lifetimes are of the order of 10^{-10} seconds. The expected lifetime if the decay proceeded by a strong interaction would be of the order of 10^{-23} seconds.

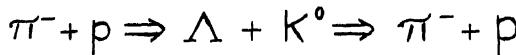
The first successful assumption made to explain these facts was

Table II
Conservation laws and their validity range.

	Strong Interactions	Electromagnetic Interactions	Weak Interactions
Conserved	$I^2, I_3(S)C,$ P, T	$I_3(S)C, P, T,$ γ_5	$C P, T, \gamma_5$
Not Conserved	γ_5	I^2	$I^2, I_3(S), C, P$

the law of associated production, due to Pais (1952). This law states that strange particles are generated only in pairs, and the strong interaction applies to this production only. The decay, which occurs where the particles are greatly separated, thus cannot go via strong interactions; it can proceed only through weak interactions, with correspondingly longer lifetimes.

Gell-Mann and Nishijima in 1953 achieved a much more detailed theory by extending the concept of isotopic spin conservation to the strange particle interactions. As an example for seeing the necessity of this extension, consider the virtual process



which should contribute to the pion-nucleon interaction. If isotopic spin were not conserved in the production of Λ and K^0 one would, from this equation, expect that the pion-nucleon interaction is not charge independent. One is therefore led to assign to all the new particles an isotopic spin quantum number in such a way that at every step these quantum numbers are conserved.

To make the necessary generalization, one first asks: How is the charge Q of the nucleon related to isotopic spin? It can be seen from the assignment for the proton and neutron that the relation is in this case $Q/e = I_3 + 1/2 n$, where n is the nucleon number. This formula can also be applied to the antiparticle; in that case, the charge and nucleon number both change sign, and the eigenvalue for the I_3 component of the antiparticle must therefore have a sign opposite to that of the particle. The same formula also holds for the pion and for any pion-nucleon system, because the pions have baryon number $n = 0$, and $Q/e = I_3$.

In the most general expression of this type, Q/e must always be linear in I_3 , since in a system containing more than one particle, both Q/e and I_3 add algebraically. Furthermore, in the expression

$$Q/e = \alpha I_3 + \frac{1}{2} Y \quad (1)$$

we must assign $\alpha = 1$. This assignment is required because, for each value of total isotopic spin I there should exist $2I + 1$ different charge states, successively differing from each other by one unit of charge. The parameter Y is thus available to describe the different charge multiplets.

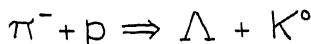
It is most natural to assign to the Λ particle the isotopic spin values $I = 0$, $I_3 = 0$, since no charged counterpart to this particle exists. Therefore Y must be zero for this particle. Thus Y cannot be simply n as in the nucleon case, since $n = 1$ for the hyperons. One may, however, write

$$Y = n + S \quad (2)$$

and assign the value $S = -1$ to the Λ particle. S is called the strangeness quantum number. One could equally well use Y alone for the description of the particle in this equation, but this separation into n and S is more convenient.

It is immediately apparent that Y is a conserved quantity, since in strong interactions both I_3 and Q are conserved. Since the baryon number is strictly conserved, the strangeness S must also be a conserved quantum number. Because of the strict conservation of charge and baryon number, I_3 conservation always implies S conservation, and vice versa; the two are equivalent.

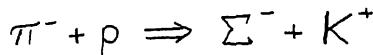
Using this general formula (1), one can assign isotopic spin values to all the strange particles. We shall begin with the K particles, and consider the reaction



In order to conserve I_3 , the K^0 particle must have $I_3 = -1/2$. The total I -spin can hence be $1/2$ or $3/2$; higher spins are not consistent with the reaction. But if the total I -spin were $3/2$, this would imply the existence of particles with $I_3 = 3/2$; this particle would necessarily be doubly charged. Such particles have never been observed; we therefore assign the value $I = 1/2$ to the K particle. Thus K^0 has the quantum number $I_3 = -1/2$, and K^+ , $I_3 = +1/2$, and from Eq. (1) one finds $Y = +1$ and $S = +1$. From this assignment it follows that the K^- particle must necessarily be the antiparticle to the K^+ ; it has $I_3 = -1/2$ and $S = -1$. Then the antiparticle to the K^0 , \bar{K}^0 , has $I_3 = +1/2$ and $S = -1$. It is also

apparent that the \bar{K}^0 must be different from the K^0 , since its I_3 component and strangeness have the opposite sign, and it will therefore behave quite differently in strong interactions.

One can similarly deduce the assignments for the Σ particle, using for example the reaction



to arrive at the assignments below:

	I_3	Y	S
Σ^+	+1	0	-1
Σ^0	0	0	-1
Σ^-	-1	0	-1

Apparently Σ^- cannot be the antiparticle of Σ^+ since both have the same strangeness.

Assignments for the Ξ particles are complicated by the fact that so few of them have been observed. The usual assignment is made on the basis of the fact that the Ξ has been seen in conjunction with two K^- mesons. This would indicate, since the production reaction involves a strangeness-conserving strong interaction, that the Ξ particle strangeness is -2 or 0 depending on whether the K 's are like or unlike particles.

From the charge formula, the corresponding I_3 values for the Ξ^- particle are then:

S	I_3
+2	$-5/2$
-2	$-1/2$

S I₃

0 -3/2

The value S = +2 would indicate the existence of at least six particles, and S = 0 at least four; in each case, some of these would necessarily be doubly charged. In order to avoid this possibility, the strangeness of the particle is taken to be -2. One then has I = 1/2, and there should also exist an uncharged particle with I₃ = 1/2, although this has not been observed as yet.²³ Table III summarizes the assignments of all particles.

Consequences of the Gell-Mann-Nishijima theory

Selection rules: With the strangeness assignment considered, the decay of the Λ , Σ and Ξ particles by strong interactions is automatically forbidden. For example, in the decays



the strangeness on the right is zero, and on the left -1. Thus, a strong interaction is not possible.

The strangeness assignment does not exclude a strong interaction between the strange particles, however, and a reaction such as

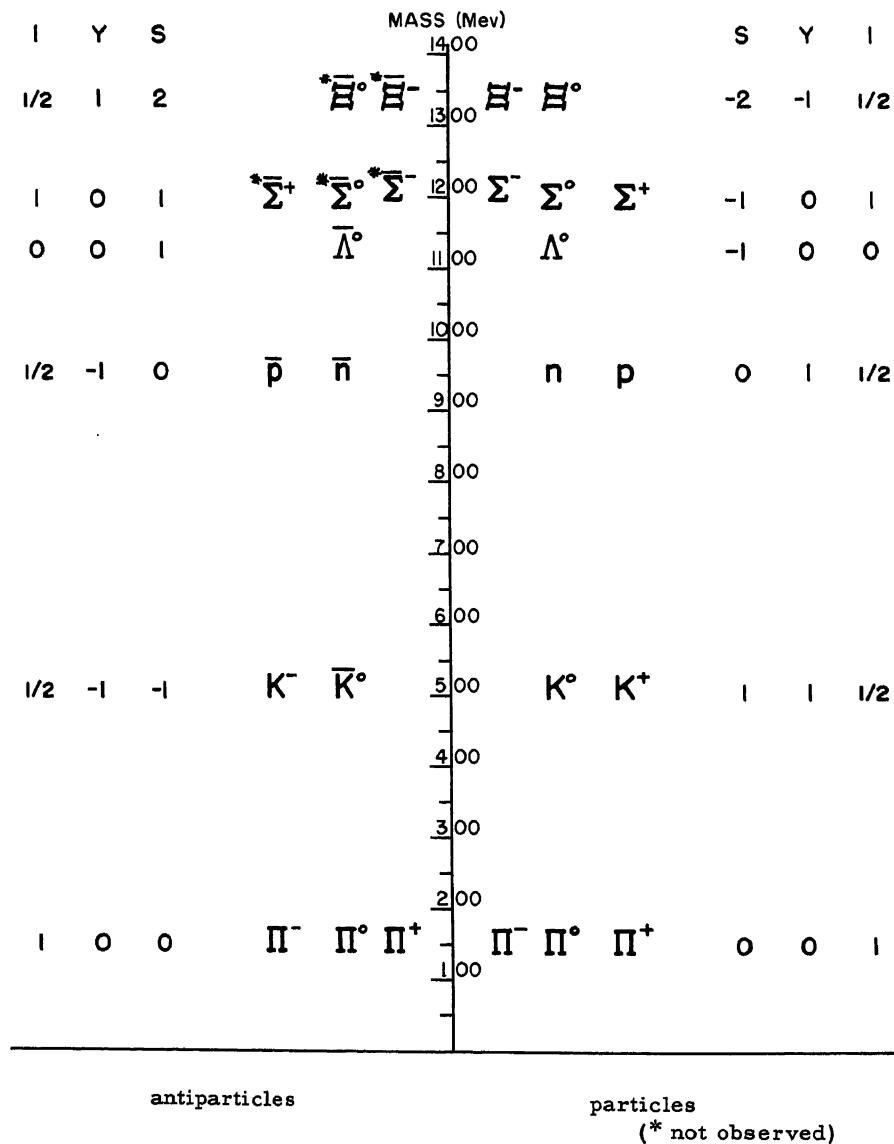


is perfectly permissible as far as the strangeness conservation is concerned. Such a reaction, however, is not allowed energetically and can therefore only occur in virtual transitions. In general, the strangeness and energy conservation together are responsible for the stability of the particle against a strong decay; some examples of this are:

<u>Reaction</u>	<u>By Strangeness Conservation</u>	<u>By Energy Conservation</u>
$n \Rightarrow p + \pi^-$	allowed	forbidden
$\Lambda \Rightarrow p + K^-$	allowed	forbidden
$\Sigma^+ \Rightarrow \Lambda + \pi^+$	allowed	forbidden
$\Lambda \Rightarrow p + \pi^-$	forbidden	allowed
$K^+ \Rightarrow \pi^+ + \pi^0$	forbidden	allowed

Table III

Strangeness and isotopic spin of strongly interacting particles. (Taken in part from Gell-Mann and Rosenfeld.)

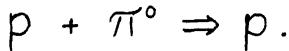


Only three cases exist where the strangeness and energy conservation allow a fast decay process. These are the electromagnetic decays:



The strangeness concept also has important consequences in the reactions of the new particles with nucleons. A case in point is the K^- meson. As we have seen, it is necessary to assign the K^- to be the anti-particle to the K^+ , and to assume that the K^0 and \bar{K}^0 are different particles; the K^- and \bar{K}^0 have strangeness -1, the K^+ and K^0 , strangeness +1. Their reactions with nucleons should thus be quite different. For reasonable energies, the K^0 and K^+ should only be capable of elastic (and, in interaction with nuclei, inelastic) and charge exchange scatterings, since no other particles have strangeness +1; the K^- and \bar{K}^0 , however, should be capable of producing hyperons. The prediction is in striking agreement with experiment. In addition, one understands why, in a beam of K particles, the number of K^+ exceeds the number of K^- ; a K^- must always be formed together with a K^+ and thus requires a higher energy than the K^+ production process $\pi^+ + n \Rightarrow \Lambda + K^+$.

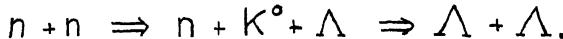
The difference between the K^0 and \bar{K}^0 can be checked by another experiment. Consider the virtual Yukawa processes



From the existence of both reactions it follows that the π^0 is the same particle as the $\bar{\pi}^0$. Suppose the K^0 and \bar{K}^0 are identical particles. By means of the virtual steps--where the last one of course violates strangeness conservation--



one could obtain the reaction



Such a process has never been observed, in spite of the fact that charge and baryon number are conserved.

Role of the electromagnetic interaction

It is perhaps conceivable that a reaction forbidden by the strangeness conservation law might become allowed through an electromagnetic interaction. That this does not happen seems to be due to a rule, called the principle of minimal electromagnetic interaction, which states that electromagnetic interactions occur only through charges and currents interacting with the electromagnetic field, and not through any other direct interaction. For example, even though the proton interacts with the electromagnetic field through its anomalous magnetic moment as well as through its charge, in any more detailed theory the anomalous moment is considered to be due to the meson cloud surrounding the nucleon, which in turn has an electromagnetic interaction only through its current.

This assumption of an electromagnetic interaction only through charges and currents implies that the interaction Hamiltonian, according to Eq. (1) contains only the I_3 isotopic spin operator, and therefore I_3 (and also S) will commute with the Hamiltonian. The electromagnetic interaction therefore conserves I_3 and so the strangeness rules hold even in the presence of electromagnetic interactions.

Cross section relations

In addition to the conservation of strangeness, the Gell-Mann-Nishijima theory postulates the conservation of total isotopic spin in strong interactions involving these particles. This conservation leads to a number of relations between various cross sections.

For example the $\Lambda^0 - p$ interaction must be the same as the $\Lambda^0 - n$ interaction, since $I = 0$ for the Λ particle, and the two systems differ only by their I_3 components. Furthermore, in the reactions

$$K^- + d \Rightarrow \Lambda + n + \pi^0 \quad \text{with cross section } \sigma_{\pi^0}$$

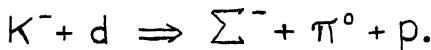
$$\text{and} \quad K^- + d \Rightarrow \Lambda + p + \pi^- \quad \text{with cross section } \sigma_{\pi^-}$$

the total isotopic spin of the left side is $1/2$, since for the deuteron $I = 0$. Constructing the wave function for total isotopic spin $1/2$ for the right-hand side, it follows directly that $\sigma_{\pi^-} = 2 \sigma_{\pi^0}$.

Another simple example is the comparison between the cross sections of the reactions

$$K^- + d \Rightarrow \Sigma^0 + \pi^- + p$$

and

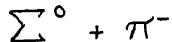
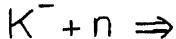
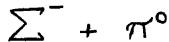


Again the right hand side must have total isotopic spin $1/2$. In this case, however, the Σ^0, π^- combination occurs with equal probability as the Σ^-, π^0 ; the two cross sections are therefore the same.

This analysis can be extended to more complicated cases: the reactions



and



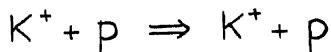
are also related through the conservation of isotopic spin. A simple relation exists for the scattering of K^- particles on target nuclei for which $Z = N$. In this case,

$$n(\Sigma^+) + n(\Sigma^-) = 2 n(\Sigma^0) \quad (3)$$

where $n(\Sigma)$ is the total number of the respective particles produced. Present experimental evidence agrees with this relation, but up to now is not conclusive enough to prove its validity.

Investigation of forces in strong interactions

As we have seen, positive K particles of moderate energy can only react with nucleons in the following ways:





That is, only elastic, inelastic and charge exchange scatterings occur in collisions with nuclei.

One may discuss the interaction of K^+ particles with nuclei in terms of the optical potential; cross section measurements may then be used to determine the strengths and relative signs of the potential. A suitable optical potential is

$$\phi = \frac{V + iW}{1 + e^{(r-6)/d}} \quad (4)$$

V is the attractive or repulsive part of the potential, W is the absorptive part, and the denominator determines the shape of the potential well.

The total and inelastic cross sections for K^+ scattering on emulsion nuclei with K^+ energies in the region of 150 Mev have been measured.^{6, 7} The experimental values are:

$$\sigma_{\text{total}} = 550 \pm 50 \text{ mb} \quad (\text{for angles larger than } 10^\circ)$$

$$\sigma_{\text{inelastic}} = 284 \pm 20 \text{ mb}$$

They can be obtained by solving the Schrödinger equation with the parameters $W \approx -10$ Mev and $V \approx -40$ or $+27$ Mev.

To decide which of the two values for V is correct, the attractive or repulsive one, one plots the differential cross section for elastic scattering as a function of angle (Fig. 2). For an attractive potential there exists around 6 degrees a destructive interference between potential and Coulomb scattering; for the repulsive potential, a corresponding constructive interference. The experimental points favor a repulsive potential $V \approx +27$ Mev. For details of procedure and results, see Ref. 6.

From the value for W one can obtain a value for the average scattering cross section $\bar{\sigma}$ for the scattering on single nucleons. The index of refraction obtained from the Schrödinger equation is

$$n = \sqrt{2m_k/\hbar^2(E-V-iW)} \quad (5)$$

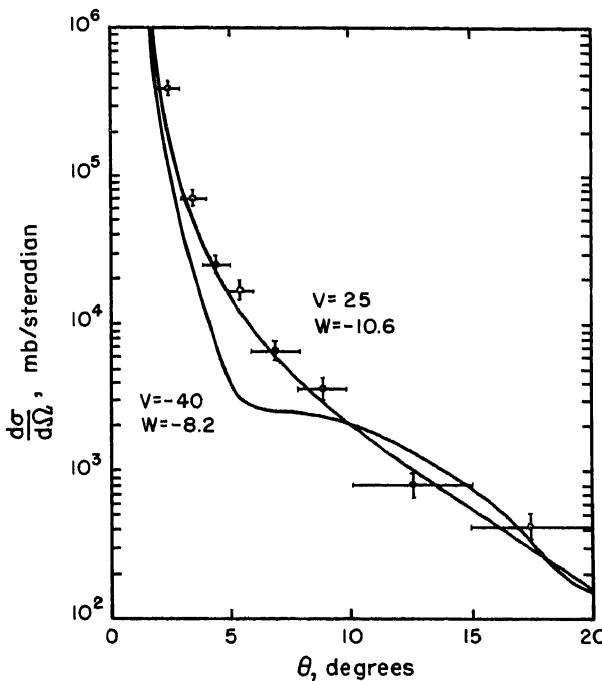


Fig. 2 Curves for differential elastic scattering cross sections of K^+ on emulsion nuclei for different values of optical potential parameters. (After Igo et al.⁶)

and, since $\rho\bar{\sigma} = \text{Im } n$, where ρ is the density of nuclear matter, we can write, calling the velocity of the K^+ particle inside nuclear matter v_K ,

$$\bar{\sigma} = -\frac{1}{\rho} \frac{W}{\hbar v_K} \frac{1}{\eta}. \quad (6)$$

The factor $1/\eta$ has been introduced in this equation to take into account the fact that the Pauli principle prohibits transitions by which the nucleons would go into occupied states. This correction factor can be calculated approximately and the final result for $\bar{\sigma}$ including this correction is:

$$\bar{\sigma} = 13 \pm 2 \text{ mb.}$$

The ratio of charge exchange scattering on nuclei to elastic and inelastic events may be used to determine the relative importance in the K-particle-nucleon system of isotopic spin 1 and isotopic spin 0 amplitudes a_1 and a_0 respectively, and hence to determine the relative magnitudes of the scattering cross sections of K particles on protons and K particles on neutrons. K^+ scattering on protons is described by a_1 alone: $\sigma_{K^+, p} = 4\pi |a_1|^2$. The elastic scattering on neutrons has the amplitude $\frac{1}{2}(a_1 - a_0)$ and the charge exchange scattering on neutrons, the amplitude $\frac{1}{2}(a_1 + a_0)$; hence the total cross section is $\sigma_{K^+, n} = 4\pi \cdot \frac{1}{2}(|a_1|^2 + |a_0|^2)$.

Experimentally the cross sections are studied using emulsion nuclei for which the number of protons is approximately equal to the number of neutrons. The ratio we are looking for, the number of charge exchange scatterings to the total number of events, is in this case

$$\frac{\text{charge exchange}}{\text{all events}} = \frac{\frac{1}{4} |a_1 - a_0|^2}{|a_1|^2 + \frac{1}{2}(|a_1|^2 + |a_0|^2)}.$$

This ratio has been measured to be about 1/5.6, which suggests that a_0 is small compared to a_1 . The neutron cross section should therefore be $\sigma_{K^+, n} \approx \frac{1}{2} \sigma_{K^+, p}$ and the average cross section is thus

$$\bar{\sigma} \approx \frac{3}{4} \sigma_{K^+, p}.$$

From K-Meson-Hydrogen scattering events one has a direct determination of $\sigma_{K^+, p}$:⁷

$$\sigma_{K^+, p} = 14.5 \pm 2.2 \text{ mb.}$$

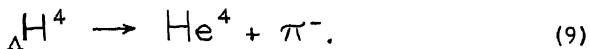
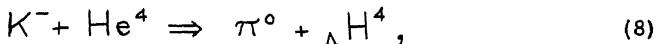
$\bar{\sigma}$ determined by this method is therefore in rough agreement with the value obtained from the imaginary part of the optical potential.

Parity of the K meson

In the same way that intrinsic parity is assigned to the pion, an intrinsic parity can be assigned to the strange particles. Because parity is not conserved in weak decays, it is not possible to determine the parity of the strange particles by studying their decays; one has to use strong interactions.

Since in strong interactions the K meson is always produced in conjunction with a hyperon, only the relative parity of, say, the Λ and the K mesons has any meaning. We shall by definition choose the parity of the Λ particle to be +1: the parities of the remaining particles, K, Σ , etc., are then experimentally measurable quantities.

The K meson parity has not been measured as yet. One possibility for a determination would be the study of the absorption of the K^- particle by He^4 , producing the hyperfragment Λ^4 , and the angular distribution of the subsequent decay;⁸



To see the various consequences, the following possibilities are discussed:

1. The spin of ${}_{\Lambda}H^4$ is zero and the parity of the K meson is positive. The intrinsic parity on the left of Eq. (8) is then positive and on the right is negative. Further, since all particles have spin zero, the total angular momentum is just the orbital angular momentum, which must be the same on both sides of the equation. Hence in this case the reaction would be completely forbidden.

2. The spin of the ${}_{\Lambda}H^4$ is zero and the parity of the K meson is negative. The same arguments apply, except that now parity is conserved and the reaction is allowed; furthermore, the angular distribution of the decay products of ${}_{\Lambda}H^4$ will be isotropic, since the spin of the ${}_{\Lambda}H^4$ is zero.

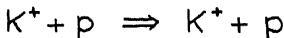
3. Similar arguments can be advanced for the case of spin 1 for the ${}_{\Lambda}H^4$, as can be seen from the following table:

Table IV

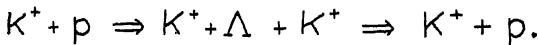
Spin ${}_{\Lambda}H^4$	Parity of the K meson	Permissible j to conserve parity	Total ang. mom.	Ang. dist. of decays
1	+	$l_K = 0$	odd	allowed
		$l_K = 1$	even	allowed
1	-	$l_K = 0$	even	forbidden
		$l_K = 1$	odd	allowed

In this table is the angle between the line of flight of the ${}_{\Lambda}H^4$ and the π^- -meson.

It is clear that a measurement of the angular distribution of decay products will yield at least an indication of the desired parity. The expected result of this measurement is not clear; there is one rather weak theoretical argument, however, which indicates that the K meson may be a particle with negative intrinsic parity. Considering the scattering



as due to a Yukawa-type interaction involving the virtual exchange of K^+ mesons,



The corresponding interaction Hamiltonian may be written in the form

$$H_{\text{int}} = g_{\Lambda K} \{ (\bar{p} O \Lambda) K^+ + (\bar{n} O \Lambda) K^0 \} + \text{herm. conj.}, \quad (10)$$

where the operator O is unity for scalar K , and $i\gamma_5$ for pseudoscalar K particles.

If one performs a perturbation calculation, an attractive force results for the scalar theory, and a repulsive one for the pseudoscalar theory. The first order perturbation calculations are in no way convincing, especially in the pseudoscalar case; with the assumption of mainly s wave scattering, however, which is experimentally indicated from the angular distribution in the K^+ scattering on protons, the scalar solution should have some qualitative validity. But the attractive potential calculated in the scalar case is contrary to experiment; hence the pseudoscalar theory is more likely to be correct.

Λ Particle-nucleon interactions

Most of the knowledge we have today about the nature of the Λ particle-nucleon interaction has come from a study of hyperfragments, nuclei in which a Λ particle is bound like a neutron. The existence of such particles is well established and the binding energies and decay schemes of many of them are known. Examples of such hyperfragments are ${}_\Lambda^4 H$, ${}_\Lambda^4 He$, ${}_\Lambda^5 He$ and ${}_\Lambda^9 Be$. Heavier hyperfragments have been observed, but not extensively enough to have been thoroughly investigated.

The binding energies of these hyperfragments can be determined from the decay products by the relation

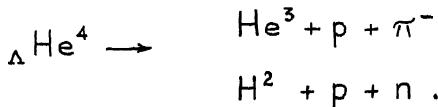
$$B_\Lambda = M_{\text{init}} + M_\Lambda - \sum_{\text{final}} M_{\text{final}} - Q, \quad (11)$$

where M_{init} and M_{final} are the masses of the initial nucleus (without the Λ) and the products of the reaction respectively, and M_Λ is the mass of the Λ particle.

It is found that the binding energy of the particle increases approximately linearly with the number of nucleons in the fragment. This is to be expected. Since the Pauli principle has no effect on the Λ particle, it is always in the lowest s state of a potential well arising from the other nucleons. The radius of the well increases with A . A simple perturbation calculation then shows that for constant nucleon density, the binding energy must increase linearly with A .

The magnitude of the observed binding energy is less than the corresponding nucleon binding energy. This is obviously the reason why the hyperfragments ${}^A\text{H}^2$ and ${}^A\text{H}^3$ do not exist, contrary to the existence of the corresponding normal isotopes, H^2 and H^3 . The existence of ${}^A\text{H}^4$ and ${}^A\text{He}^5$ does not contradict this reasoning; in these cases the Pauli principle, which prevents the binding of H^4 and He^5 , gives no restriction for the Λ particle.

The hyperfragments have both mesonic and non-mesonic decays; for example, ${}^A\text{He}^4$ decays by either of the processes



The decays are explained by the weak decay process $\Lambda \rightarrow p + \pi^-$ taking place within the nucleus. In the mesonic decays this process is a real one, and the proton carries away about 100 Mev/c of momentum. In the larger nuclei, however, such momentum states are already occupied and such a process is inhibited.

In the non-mesonic decays the process above occurs virtually; the π^- is absorbed by one of the nucleons, and the corresponding energy contributes to the proton momentum. The resultant momentum, ~ 420 Mev/c, is much greater and this decay process is therefore the preferred one in larger nuclei.

The experimental ratio between mesonic and non-mesonic decays has been used to give an argument against a high spin for the Λ particle. A high spin would lead to a strong momentum dependence of the reaction $\Lambda \rightarrow p + \pi^-$; this momentum dependence would affect the ratio between the two types of decay. Such a dependence has not been found and indeed the spin of the Λ particle turned out to be $1/2$ also by means of different methods.⁹

Theoretically it is difficult to understand the Λ binding in nuclei by the K meson coupling. The range of such a coupling is only of the order of the Compton wavelength of the K meson. In addition, the coupling strength appears to be smaller than the nucleon-pion coupling, as can be inferred from the smallness of the observed photoproduction cross section of K mesons.¹⁰ To explain the binding a strong force compatible in range and strength with the nucleon-nucleon force is necessary. A two pion exchange of the type

$$\Lambda + n \Rightarrow \Lambda + \pi^- + p \Rightarrow \Sigma^- + p \Rightarrow \Sigma^- + \pi^+ + n \Rightarrow \Lambda + n$$

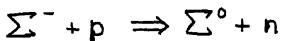
has the range of one-half of the pion Compton wavelength and is the only

relatively simple possibility, provided the coupling between Λ , Σ and pions is as strong as the pion-nucleon coupling.

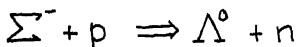
Such a force should in general be spin dependent and its effect should show up in the relative binding energies of ${}^5\text{He}$ and ${}^4\text{H}$. In ${}^4\text{H}$ the Λ particle may orient itself parallel or antiparallel to the unpaired neutron and thereby gain some additional energy. This is not possible in ${}^5\text{He}$. The measured binding energies of these nuclei indicate such a spin dependent Λ -nucleon force.¹¹

Σ particle-nucleon interactions

The Σ -nucleon interactions are similar to the Λ -nucleon interactions, as evidenced by the experimental observation that the reactions



and



have similar cross sections. This result is to be expected, since the particles have the same strangeness. The second reaction prevents the existence of Σ hypernuclei.

The hypothesis of global symmetry

The Λ -nucleon force indicates, as shown before, that the hyperons have interactions with π mesons with a strength similar to that of the pion-nucleon interaction. The K meson interactions, on the other hand, according to the small photoproduction cross section, seem to have smaller coupling constants. Gell-Mann⁸ suggested, therefore, that the "very strong" pion couplings which are allowed by strangeness conservation possess a high, so-called global, symmetry. This symmetry should be of the kind that, if the "medium strong" K particle interactions could be switched off, all the hyperons and nucleons would have equal masses and thus would form a completely degenerate system of particles. This idea thus requires that the coupling between Ξ^- , Ξ^0 and the pions must be identical with the Yukawa coupling between n, p, and the pions. The couplings between the Σ and Λ particles and the pions must also have this form; a slight manipulation is necessary to accomplish this, however, since Σ and Λ have integral isotopic spin. The combinations Σ^+ , $Y^0 = \frac{1}{\sqrt{2}}(\Lambda^0 - \Sigma^0)$ and $Z^0 = \frac{1}{\sqrt{2}}(\Lambda^0 + \Sigma^0)$, Σ^- each behave like the p, n, combination, and can therefore be coupled with the π meson field in the same way as the nucleons. Note that global symmetry can only be correct if all the baryons have spin 1/2 and equal parity.

The complete degeneracy is removed by the K particle couplings, which are assumed to be responsible for the mass differences between the

baryon multiplets. As long as one can consider the latter coupling to be a small perturbation, by global symmetry there should exist relations between strange particle interaction matrix elements and nucleon-pion matrix elements. These relations may be of use in actual calculations.

III. Weak Interactions

We have already mentioned the conservation laws applying to the weak interactions. Before amplifying in general on the implications these laws carry, and before discussing the interactions in more detail, we shall outline the interesting special case of the decay of the neutral K meson, where the CP conservation law has particular consequences.

Decay of the neutral K meson

The K meson, called the θ^0 particle, can decay into two pions by the reactions

$$K^0 \rightarrow \pi^+ + \pi^-$$

and

$$K^0 \rightarrow \pi^0 + \pi^0.$$

The right sides of these reactions are however, eigenstates of the CP operation, with eigenvalues + 1. Thus, due to this weak interaction, the transformation of a K^0 into its antiparticle \bar{K}^0 has a certain probability of occurrence:

$$K^0 \rightarrow \pi^+ + \pi^- \rightarrow \bar{K}^0.$$

In weak interactions CP is conserved; in order to discuss the decay, one forms eigenstates of this operator. For a K^0 at rest one has, by a proper choice of the phases, the relations

$$CP|K^0\rangle = |\bar{K}^0\rangle, \quad CP|\bar{K}^0\rangle = |K^0\rangle. \quad (12)$$

The combinations

$$K_1^0 = \frac{1}{\sqrt{2}} \{ |K^0\rangle + |\bar{K}^0\rangle \} \quad (13)$$

and

$$K_2^0 = \frac{1}{\sqrt{2}} \{ |K^0\rangle - |\bar{K}^0\rangle \}$$

then form eigenstates of CP, with eigenvalues 1 and -1, respectively. The only particle in this scheme capable of decaying into two pions is K_1^0 ; the K_2^0 must decay into three pions or by some other mode having an eigenvalue of CP equal to -1.

A beam of K^0 particles generated by a strong interaction consists initially, according to Eq. (13), of equal numbers of K_1^0 and K_2^0 particles,

$$|K^0\rangle = \frac{1}{\sqrt{2}} \{ |K_1^0\rangle + |K_2^0\rangle \} \quad (14)$$

and must therefore have two different lifetimes corresponding to the K_1^0 and the K_2^0 decays. This has been verified experimentally; the K_1^0 decay (into two pions) has a lifetime¹² of $0.99 \pm 0.12 \times 10^{-10}$ sec. while the K_2^0 particle's lifetime is $9.0^{+6}_{-7} \times 10^{-8}$ sec.¹¹

If a beam of K^0 particles travels for a sufficient time the K_1^0 part of it decays; the K_2^0 part remains for a longer time, and consists of equal numbers of K^0 and \bar{K}^0 particles with the special phase relation given in (13). A "stale" beam of neutral K's can therefore produce strong reactions typical of \bar{K}^0 particles. Experimentally, reactions of the type shown in Fig. 3 have been observed; here the particle, originally a K^0 , acts as a \bar{K}^0 .

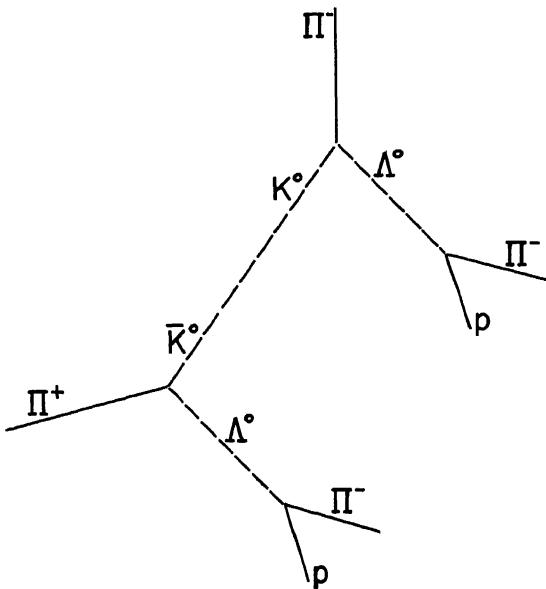


Fig. 3 K^0 production process followed by a \bar{K}^0 reaction with a proton illustrating the change of a K^0 into a \bar{K}^0 (see text).

K_1^0 and K_2^0 should have exactly equal masses as long as only strong interactions are considered; they are merely linear combinations of particle and antiparticle. But they differ in their weak interactions, and thus a slight mass difference corresponding to the different self-energies should exist. The magnitude of this mass difference may be of the order

$$\Delta m \approx \frac{\gamma}{\tau_{K_1^0}} = 6 \times 10^{-12} \text{ Mev.}$$

A particle which at time $t = 0$ is a K^0 will therefore have a time dependent wave function given by

$$|\psi(t)\rangle = \frac{1}{\sqrt{2}} |K_1^0\rangle e^{-im_1 t - \Gamma_1 t/2} + \frac{1}{\sqrt{2}} |K_2^0\rangle e^{-im_2 t - \Gamma_2 t/2} \quad (15)$$

where m_1 and m_2 are the masses of K_1^0 and K_2^0 , respectively, and Γ_1 and Γ_2 the corresponding decay constants.

The probability that after a time t the particle is still a K^0 is then given by the relation

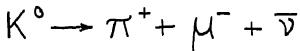
$$| \langle K^0 | \psi(t) \rangle |^2 = \frac{1}{4} \{ e^{-\Gamma_1 t} + e^{-\Gamma_2 t} + 2 e^{-(\Gamma_1 + \Gamma_2)t/2} \cos(m_1 - m_2)t \} \quad (16)$$

and the corresponding probability that the particle is a \bar{K}^0 is given by the relation

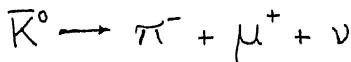
$$| \langle \bar{K}^0 | \psi(t) \rangle |^2 = \frac{1}{4} \{ e^{-\Gamma_1 t} + e^{-\Gamma_2 t} - 2 e^{-(\Gamma_1 + \Gamma_2)t/2} \cos(m_1 - m_2)t \} \quad (17)$$

The oscillatory time dependence of these probabilities in principle affords a method of measuring the slight mass difference between the K_1^0 and K_2^0 if this mass difference is of the order given above.

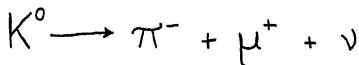
There are theoretical arguments which we shall discuss later that in the leptonic decay modes of neutral K particles the processes



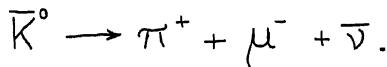
and



do not occur. Instead, the decay should be



and

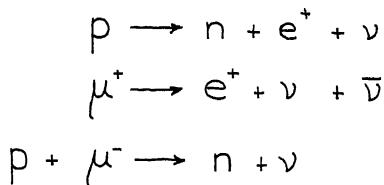


The number of μ^+ and μ^- is therefore a measure of the probability (Eqs. (16) and (17)), and should vary accordingly.¹³

The neutral K decay is of course not typical; other (charged) mesons cannot decay in such a peculiar fashion, since they are not neutral systems, and hence not eigenstates of CP.

General aspects of weak interactions

Weak interactions were known long before the discovery of strange particles. The couplings involved in the four fermion interactions



were known to have about equal strength, and a so-called "universal Fermi interaction" had been postulated. This universality is symbolized by the Puppi triangle shown in Fig. 4.

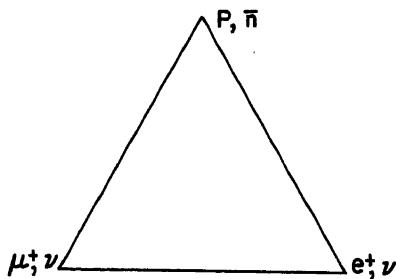


Fig. 4 The Puppi triangle

In this diagram the vertices represent, and are labelled by, a pair of particles. The sides of the triangle represent the interaction between the particles at the vertices; the equal lengths of the sides indicate the equal strength and form of the interactions. Notice that no antineutrinos appear in the triangle. The decision as to which lepton is a particle and which the antiparticle is to some extent a matter of definition. It is desirable, however, to attempt to define the particles and antiparticles in such a way that a law of lepton conservation can be stated. As a starting point, one thus defines the electron to be a particle, the positron to be an antiparticle, and, consistent with the conservation law, the neutrino appearing in the reaction

$$p \rightarrow n + e^+ + \nu$$

is also defined to be a particle.

In the case of μ decay $\mu^+ \rightarrow e^+ + \nu + \bar{\nu}$, we can deduce from the spectrum shape of the decay that the two neutrinos emitted must be different particles--neutrino and antineutrino. In order that the lepton conservation law hold in this case, we define the μ^- to be a particle like the electron; the μ^+ must then be the corresponding antiparticle.

The law of conservation of leptons which we have constructed by these definitions is not, however, without its experimental consequences. For example, in the reactions

$$\pi^+ \rightarrow \mu^+ + \nu, \quad K^+ \rightarrow \mu^+ + \nu$$

the conservation law requires that the massless particle be a neutrino and not an antineutrino. Since we know that a neutrino has its spin pointing opposite to its momentum (see the two-component neutrino theory below), we infer that in a system in which the pion is at rest the μ^+ spin is aligned in the same way relative to its momentum, in order to conserve angular momentum. The longitudinal polarization of the μ^+ meson--as inferred from measurements on μ^+ decay--therefore gives evidence for the validity of the law of conservation of leptons.

The pion decay is qualitatively explained by the fact that the p, n pair is strongly coupled to the pion field:

$$\pi^+ \Rightarrow p + \bar{n} \rightarrow \mu^+ + \nu.$$

This decay suggests a generalization of the triangle to include the strange particle decays. We have seen that the hyperons also interact, if strangeness is conserved, by strong couplings with pions; then virtual processes like

$$\pi^+ \Leftrightarrow \Sigma^+ + \bar{\Lambda}$$

should exist. The pair $\Sigma^+, \bar{\Lambda}$ can then be considered to somehow be connected with the pn apex. We hence assume that all baryon pairs with total strangeness zero have their weak decays represented by the Puppi triangle and appear at the pn apex. (See Fig. 5.)

To complete the generalization to strange particles we must also account for the observed process

$$K^+ \rightarrow \mu^+ + \nu.$$

The addition of all pairs of particles with strangeness zero to the pn apex suggests that a similar treatment be made for the particles strongly coupled to the K^+ meson; the total strangeness here, however, must be +1. This generalization adds a fourth leg to the scheme (now a tetrahedron), and it is most natural to allow couplings from this vertex not only to the μ, ν vertex, but to all others. The complete construction is shown in Fig. 5. In this scheme decays take place by a series of strong (virtual) interactions combined with one weak interaction; for example, the decay of K^+ mesons into pions is explained qualitatively by the reactions

$$K^+ \Rightarrow p + \bar{\Lambda} \rightarrow p + \bar{n} \Rightarrow \text{pions.}$$

Because parity is not conserved in the weak four fermion coupling, the earlier puzzle that the K^+ particle can decay into two or three pions is thus resolved.

It might be expected for the sake of symmetry that still another branch in which the hyperon pairs would have total strangeness -1 should be added to this scheme. Such an addition is not included for two reasons: first, it is not necessary to explain the observed decays; and second, it would lead to decays in which the strangeness changes by two units.

Pairs like $\Xi^-, \bar{\Xi}^0$ would then be coupled to pairs like $\bar{\Sigma}^+, n$; such a branch would imply that the process

$$\Xi^- \rightarrow \Sigma^0 + \bar{\Sigma}^+ + n \Rightarrow \pi^- + n$$

could proceed by a weak interaction. This process has not been observed, a fact that might be due to the strangeness change of two units in this transition.

If the exclusion of the strangeness -1 branch of this scheme is valid, the leptonic modes of the K decay, which we discussed earlier, are predicted to be only

$$K^0 \rightarrow \mu^+ + \nu + \pi^-$$

or

$$K^0 \rightarrow e^+ + \nu + \pi^-,$$

and decays into positive pions,

$$K^0 \rightarrow \mu^- + \bar{\nu} + \pi^+$$

or

$$K^0 \rightarrow e^- + \bar{\nu} + \pi^+$$

are excluded.

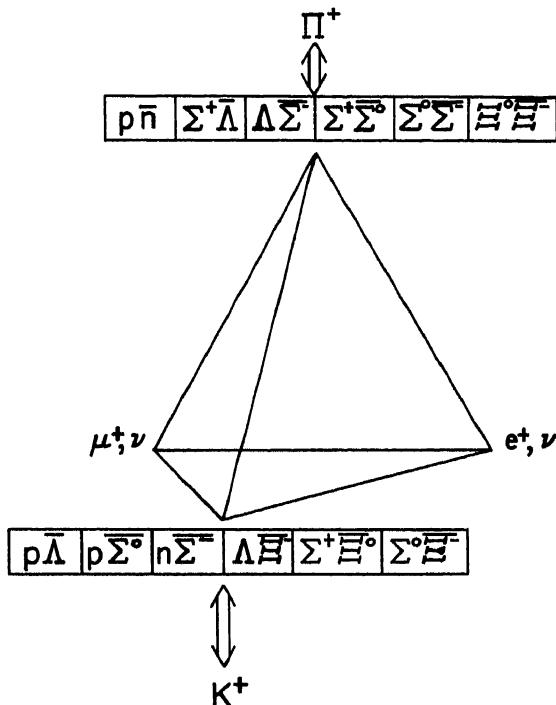


Fig. 5 Generalization of the Puppi triangle:
the tetrahedron scheme.

The tetrahedron scheme is capable of describing all the known weak decays, and provides, therefore, a good qualitative description of the couplings in weak interactions.

β decay and the two-component neutrino

To investigate in more detail the interaction which the sides of the tetrahedron scheme are assumed to represent, we shall discuss briefly the best known weak interaction, nuclear beta decay. There is no fundamental theory of the four fermion interaction, but the phenomenological theory due to Fermi has had excellent success in describing the observed effects. That such a description is so successful is due to the small interaction constant; only first order terms must be considered.

The theory states that the amplitude for the occurrence of a decay is proportional to the products of the four fields involved (the proton, neutron, electron, and neutrino wave fields) all taken at the same space points. The interaction Hamiltonian is thus given by

$$\begin{aligned} H_\beta = & \sum_i g_i (\bar{\psi}_p(x) O_i \psi_n(x)) (\bar{\psi}_e(x) O_i \psi_\nu(x)) \\ & + \sum_i g'_i (\bar{\psi}_p(x) O_i \psi_n(x)) (\bar{\psi}_e(x) O_i \gamma_5 \psi_\nu(x)) + \text{Hermitian conjugate} \end{aligned} \quad (18)$$

where

$$\bar{\psi} = \psi^\dagger \gamma_5.$$

The O_i are operators constructed from the Dirac γ matrices to insure that the interaction Hamiltonian is a scalar (or a pseudoscalar, since parity need not be conserved). The possible operators O_i are chosen so that $\bar{\psi}_p O_i \psi_n$ and $\bar{\psi}_e O_i \psi_\nu$ have the properties under Lorentz transformation of one of the five invariant quantities: scalar, vector, tensor, axial vector, or pseudoscalar. The coupling constants g_i and g'_i are real by CP invariance.

Detailed experiments performed in the last year indicate that only the vector and axial vector terms contribute to the interaction; values of the corresponding coupling constants, g_v and g_A have been found to be

$$(g_v^2 + g_A'^2)^{1/2} = (1.41 \pm 0.01) \cdot 10^{-49} \text{ erg-cm}^3$$

$$g_A = -\lambda g_v ; \lambda = 1.20 \pm 0.08$$

and

$$g'_v \simeq g_v , \quad g'_A \simeq g_A .$$

Using $O_v = \gamma_\mu$ and $O_A = i\gamma_\mu\gamma_5$ ($\gamma_5 = \gamma_1\gamma_2\gamma_3\gamma_4$) and choosing a representation in which the γ matrices are Hermitian, the Hamiltonian can be written in the form

$$H_\beta = \sum_\mu g_v (\bar{\Psi}_p \gamma_\mu (1 + \lambda\gamma_5) \Psi_n) (\bar{\Psi}_e \gamma_\mu (1 + \gamma_5) \Psi_v) + \text{c.c.} \quad (19)$$

This interaction Hamiltonian summarizes all that is experimentally known about the interaction.¹⁴ It is conceivable that other terms may be present to the degree to which the experimental values are uncertain, but the theoretical arguments which follow make large additional contributions highly improbable.

Let us briefly discuss the neutrino field. It is a property of massless particles that the operator γ_5 commutes with the Dirac Hamiltonian; in fact, an eigenstate of γ_5 with eigenvalue +1 (positive chirality state) describes a particle with its spin pointing opposite to its momentum. If in every interaction only a particular eigenstate of γ_5 is coupled, the result is equivalent to a reduction from a four-component to a two-component field. It was this type of coupling which Lee and Yang postulated in their two-component theory of the neutrino.¹⁵

It is more convenient, however, to use the four-component notation. To select the above mentioned coupling the neutrino field appears multiplied by the projection operator $1/2(1 + \gamma_5)$. The two-component theory is thus equivalent to the invariance requirement of the Hamiltonian under the transformation $\psi \rightarrow \gamma_5 \psi$.

From a theoretical standpoint it is very satisfactory, that this invariance which holds for the Hamiltonian of the free neutrino is thus extended to all the interactions in which the neutrino field appears. As a special consequence of the γ_5 invariance (which is also called chirality invariance) it follows that the neutrino in spite of its interactions remains strictly massless. Experimentally, the two-component theory of the neutrino is well established.

In the four-fermion interactions indicated in the Puppi triangle, the strength of the interactions are at least approximately equal, in spite of the fact that the particles involved in the μ decay are quite different from the heavy particles undergoing nuclear β decay. This situation suggests that the masses of the fermions are not relevant to the form and strengths of the weak interactions. It is then a plausible hypothesis, to assume that the chirality invariance, which applies to the neutrino interactions, may also hold for the weak interactions of each of the other particles.⁵ In other words, it is postulated that the special symmetry which holds for the neutrino is typical for the weak interaction and holds for all particles involved. This generalized γ_5 invariance obviously does not

extend to the mass terms in the free particle part of the Hamiltonian; one can require only the interaction Hamiltonian to exhibit the invariance. This is analogous to the isotopic spin invariance; neither is complete, both hold strictly only for special interactions. The chirality invariance holds for weak and electromagnetic interactions and is violated by strong interactions and by the mass terms (which may or may not result from strong interactions). There are striking similarities between electromagnetic and weak interactions: both have vector couplings; in both cases the coupling constants are universal, independent of the masses of the particles and both couplings violate the isotopic spin symmetry. A special consequence of the $\frac{1}{2}$ invariance principle for the electromagnetic coupling is that it rules out a direct electromagnetic coupling of particles through a Pauli term, because the so-called Pauli moment violates the invariance.

If one constructs the general β -decay interaction according to Eq. (18), and requires the complete chirality invariance, the scalar, tensor, and pseudoscalar terms contribute nothing and the V, A interactions remain, with opposite signs and equal magnitude. This is just the experimental β interaction, Eq. (19), but with $\lambda = 1$. One is thus inclined to believe that the weak interaction has the exact form V-A, in accord with the chirality invariance principle. The deviation of λ from 1 may find its explanation through the strong meson nucleon interaction, which could lead to a difference between the interaction Hamiltonian for the bare particles and the effective Hamiltonian for the physical nucleons which are surrounded by their meson clouds. (See the discussion below.)

μ Decay

The fact that in μ decay the interaction turned out experimentally as well as theoretically to be a V, A interaction is encouraging from the point of view of the universal Fermi interaction. The β -decay interaction is then consistent with the μ -decay; in the latter case, a neutrino and anti-neutrino are involved, and with no assumption other than the two-component neutrino all couplings except V-A and $(S + \text{const.} \times T) - P$ can be excluded. In addition, the measurement of the spin direction of the decay electron¹⁶ shows that V-A is the correct interaction, consistent with the theoretical requirement of chirality invariance of the interaction Hamiltonian. The Hamiltonian is therefore given by

$$H_\mu = g_\mu \sum_\lambda (\bar{\Psi}_\nu \gamma_\lambda (1 + \gamma_5) \Psi_\mu) (\bar{\Psi}_e \gamma_\lambda (1 + \gamma_5) \Psi_e) + \text{h.c.} \quad (20)$$

From the known μ -meson lifetime the coupling constant in this interaction agrees within the error limit of 1% with the coupling constant determined from the β decay of 014 .

Δ decay

Two legs of the tetrahedron scheme $p\bar{n} \rightarrow e^+\nu$ and $\mu^+\nu \rightarrow e^+\nu$

are thus identical in strength and form. This might be taken as an indication that the other interactions occurring in the scheme are also of the same form, as required by the assumption of chirality invariance, and the idea of a universal interaction.

There is already substantial evidence that the interaction represented by the side connecting the strangeness 0 vertex to the strangeness +1 vertex has this form. The evidence comes from the asymmetry observed in the Λ decay

$$\Lambda \rightarrow p + \pi^-$$

A consequence of the non-conservation of parity in this decay is that the proton emission is asymmetric with respect to the spin direction of the Λ particle.

The Λ decay may be described phenomenologically by an interaction of the form

$$H_\Lambda = F \phi_\pi (\bar{\Psi}_p (1 - r \gamma_5) \Psi_\Lambda) + i f/m_\pi \sum_\lambda \frac{\partial \phi_\pi}{\partial x_\lambda} (\bar{\Psi}_p \gamma_\lambda (1 + s \gamma_5) \Psi_\Lambda). \quad (21)$$

Corresponding to the β decay, no derivatives of the proton and Λ particle wave functions are included. F , f , r and s are real constants (the reality is imposed by CP invariance). Because the s 1/2 and p 1/2 meson-nucleon phase shifts are small in the corresponding energy region, one may regard the particles involved as free particles. A partial integration of the last term, using the Dirac equation for the proton and the Λ particle, then shows that the second term may be brought into the form of the first one. The first part of this first term then describes the amplitude for a transition of the π meson into the p 1/2 state relative to the proton; the γ_5 part in the first term describes the transition into the s 1/2 state. The relative amplitudes for these transitions are easily calculated, using

$$\Psi_p \sim (1 + \frac{\vec{\alpha} \cdot \vec{p}_p + \beta m_p}{E_p}) \chi_p, \quad \Psi_\Lambda = \chi_\Lambda \quad (22)$$

where χ_p and χ_Λ denote the spin function of p and Λ respectively. Then

$$(\bar{\Psi}_p (1 - r \gamma_5) \Psi_\Lambda) \sim \langle \chi_p | 1 + m_p/E_p - r(\vec{\sigma} \cdot \vec{p}_p/E_p) | \chi_\Lambda \rangle, \quad (23)$$

and the asymmetry parameter α for the proton emission from polarized Λ particles is thus

$$\alpha = -\frac{2z}{1+z^2} \quad , \quad \text{where} \quad z = r \frac{p_p}{E_p} \left(1 + \frac{m_p}{E_p}\right)^{-1}.$$

This asymmetry parameter is measured to be $|\alpha| \geq 0.77^{17}$. No upper limit is given because the degree of polarization of the particle (perpendicular to the plane of production in the strong interaction) is not known. Using this experimental value, r is found to be large: $7.7 \leq r \leq 48$.

This large value can easily be understood from the γ_5 invariance principle, or equivalently, from an intermediate V-A interaction in the corresponding branch of the tetrahedron. The γ_5 invariance requires $F = 0$ and $S = 1$ in Eq. (21). However, because of the Dirac equation (which, through its mass terms, allows a transformation into the form of the first term), one may use the simpler first term instead, and a comparison shows that if this is done, r must have the value

$$r = \frac{m_\Lambda + m_p}{m_\Lambda - m_p} = 11.6$$

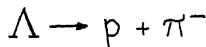
in agreement with the large experimental value.

A comparison of the strength of this interaction with that for still a fourth leg of the tetrahedron can also be made, which avoids the complications of the intermediate strong couplings. The idea is to compare directly the magnitude of the coupling constant f in Eq. (21) with the analogous coupling constant describing the $\pi^+ \rightarrow \mu^+ + \nu$ decay.

In this decay the γ_5 invariance requires the effective interaction to be of the form

$$H_{\pi \rightarrow \mu + \nu} = i \not{d}/m_\pi \sum_\lambda \frac{\partial \phi_\pi}{\partial x_\lambda} (\bar{\psi}_\mu \gamma_\lambda (1 + \gamma_5) \psi_\nu). \quad (24)$$

The partial mean life of the decay mode



is, from Eq. (21),

$$\frac{1}{\tau_{\Lambda \rightarrow p + \pi^-}} = \frac{f^2}{4\pi} 2p_p \frac{(m_\Lambda - m_p)^2 + p_p^2}{m_\pi^2}; \quad (25)$$

the corresponding lifetimes for the decay $\pi^+ \rightarrow \mu^+ + \nu$, from Eq. (24), is

$$\frac{1}{\tau_{\pi \rightarrow \mu^+ \nu}} = \frac{d^2}{4\pi} m_\pi \left(\frac{m_\mu^2}{m_\pi^2} \right) \left(1 - \frac{m_\mu^2}{m_\pi^2} \right)^2. \quad (26)$$

Using the experimental values¹⁸

$$\tau_{\Lambda \rightarrow p + \pi^-} = (4.1 \pm 0.5) \times 10^{-10} \text{ sec.}$$

and

$$\tau_{\pi \rightarrow \mu^+ \nu} = (2.56 \pm 0.05) \times 10^{-8} \text{ sec.}$$

one finds

$$\frac{f^2}{4\pi} \simeq 3.8 \times 10^{-15} \quad \text{and} \quad \frac{d^2}{4\pi} \simeq 1.8 \times 10^{-15}$$

in rough agreement with the assumption of a universal coupling strength.

Another example of this agreement is found in the Σ^- decay. One can calculate a coupling constant h in analogy to f in Eq. (25). One finds for this constant

$$\frac{h^2}{4\pi} \simeq 1.9 \times 10^{-15}.$$

Effects of strong couplings on the form of the weak interaction

It has already been mentioned that the interaction Hamiltonian for the bare particles, which is supposed to have the strict γ_5 invariance, may differ from the effective Hamiltonian for the physical particles due to the effect of the strong interactions (which do not show this invariance). It is therefore surprising that the vector coupling constants governing β decay and μ decay are in such striking agreement. Feynman and Gell-Mann¹⁹ have explained this by the assumption that in the vector part of the β interaction the vector current of the nucleons

$$\bar{\psi}_p \gamma_\nu \psi_n = \bar{\psi} \gamma_\nu \tau^+ \psi$$

is replaced by the total current, which obeys a conservation law. This means essentially the addition of meson currents like $[\vec{\phi} \times \partial \vec{\phi}, \vec{\phi}]_+$ to

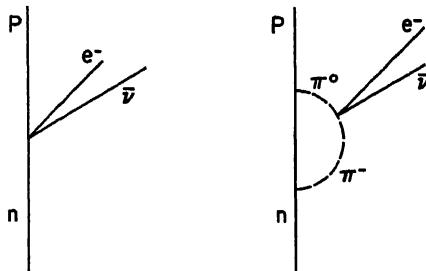
the above current. The arrows and the + sign refer to isotopic spin components, ϕ being the meson field. The conservation of this total current then assures that the observed vector coupling constant g_V is independent of the strength of the meson-nucleon coupling, in strict analogy to the independence of the charge $+e$ from the kind of meson cloud around the nucleons. If this assumption is correct, it is clear that the coupling strength for μ decay, where no virtual π' mesons are involved, is the same as the strength of the vector coupling in nuclear β decay, where the nucleons are strongly coupled to the π' meson. The vector part of the β interaction in isotopic spin notation is thus

$$g_V \sum_{\lambda} \{ \bar{\psi} \gamma_{\lambda} \tau^+ \psi + i[\vec{\phi} \times \frac{\partial}{\partial x_{\lambda}} \vec{\phi}]_+ \} (\bar{\psi}_e \gamma_{\lambda} (1 + \gamma_5) \psi_e). \quad (27)$$

The second term describes the real or virtual disintegration

$$\pi^- \rightarrow \pi^0 + e^- + \bar{\nu}.$$

The two contributions to the nuclear β decay may be illustrated by the diagrams:



One knows from electrodynamics that even though the coupling constant e^+ of a proton is not affected by the meson cloud, the meson current gives rise to the anomalous magnetic moments of the nucleons. Phenomenologically, the electromagnetic interaction of nucleons can be written as the sum of two terms, the current interaction and the anomalous magnetic moment interaction:

$$H_{\gamma_{eff}} = e \sum_{\mu} \left\{ (\bar{\psi} \gamma_{\mu} \tau_3 \psi) + \frac{\mu_p - \mu_n}{2M} \sum_{\nu} (\bar{\psi} \sigma_{\mu\nu} \tau_3 \psi) \frac{\partial}{\partial x_{\nu}} \right\} A_{\mu}. \quad (28)$$

This formula contains only the isotopic vector part of the electromagnetic interaction; A_{μ} denotes the vector potential, $\mu_p - \mu_n = 3.7$ and M is the nucleon mass.

Because the β -decay vector current is, apart from a different component of the I-spin vector, exactly the same as the current coupled in Eq. (28), we have a complete analogy between the two interactions and the effective vector interaction for the nuclear β decay thus becomes²⁰

$$g_V \sum_{\mu} \left\{ \bar{\psi} \gamma_{\mu} \tau^+ \psi + \frac{\mu_p - \mu_n}{2M} \sum_{\nu} (\bar{\psi} \sigma_{\mu\nu} \tau^+ \psi) \frac{\partial}{\partial x_{\nu}} \right\} (\bar{\psi}_e \gamma_{\mu} (1 + \gamma_5) \psi). \quad (29)$$

The second term is of the order of E_0/Mc^2 , where E_0 is the total transition energy, and thus is very small. This term gives rise to small effects in the shape of the β spectrum of allowed transitions and to the β - γ angular correlations in β transitions followed by γ -rays. Up to this time its existence has not been definitely proved, although there is an indication for it.²¹

Up to now only the renormalization of the vector part of the interaction has been considered. An analogous approach for the axial vector part, however, is not possible, because no conservation law holds for the axial vector current. The corresponding coupling constant g_A will thus in general be affected by the existence of strong couplings. This seems to be the reason for the deviation of λ from one in Eq. (19), although up to now no successful calculation of λ has been made to justify this statement.

The effective Hamiltonian from Eq. (29), together with its axial vector counterpart, contrary to the initial interaction Hamiltonian (Eq. (27) with its axial vector part), no longer has the γ_5 invariance property. This is to be expected, since the π -meson coupling with nucleons violates this symmetry. Furthermore, Goldberger and Treiman²² have shown, using dispersion relation techniques, that in the effective Hamiltonian other terms appear through the effect of the strong interactions. These terms are, however, small for the small momentum transfer in β decay; they might be appreciable, for example, in μ capture or leptonic decays of hyperons. Such terms have not been considered in the effective Hamiltonians in the previous sections.

Inconsistencies in the universal Fermi interaction

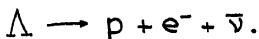
In the previous section it has been shown that the tetrahedron scheme provides a good qualitative understanding of the weak decays and to some extent even a quantitative one. It should, however, be pointed out that not all the available evidence is consistent with this scheme if taken too literally. Several of these inconsistencies follow.

The ratio of the number of π mesons decaying into electrons to the number decaying into μ mesons is independent of the strong interactions involved. For the electron decay one just may use formula (26), replacing m by m_e . The ratio is then

$$\frac{m_e^2}{m_\mu^2} \cdot \frac{(1 - \frac{m_e^2}{m_K^2})^2}{(1 - \frac{m_\mu^2}{m_K^2})^2} \simeq 1.3 \times 10^{-4}$$

The experimental upper limit for this ratio is, however, in some disagreement with the above number.*

Also, from the tetrahedron scheme one should expect lepton decays of the hyperons, for example, the decay



Using the V-A interaction and the β -decay coupling constant, the partial lifetime for this decay should be $\tau \simeq 10^{-8}$ sec. The experimental upper limit for this number is off by approximately one order of magnitude.

Another difficulty is the absence of an asymmetry in the decays of Σ^- and Σ^+ , which would be expected in analogy to the asymmetry found in the Λ decay, although here perhaps, the strong interaction process may not produce a sufficiently large polarization of these particles so that an asymmetry can be observed.

* Note added in proof: the $\pi^- \rightarrow e^- + \nu$ decay has been detected at CERN (private communication). The experiment is consistent with the theoretical ratio given above, thus removing the inconsistency.

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SOME ASPECTS OF THE STATISTICAL-MECHANICAL THEORY OF IRREVERSIBLE PROCESSES*

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I. General Features of Quasi-Thermodynamical Theory

It is sometimes said that thermodynamics is not really dynamics but is rather thermostatics, because it can give quantitative descriptions only for equilibrium states or for quasi-static processes. In the last ten years, progress has been made along lines to extend thermodynamical treatment to a wider domain of physical processes than that of the quasi-static processes. Excellent summaries of this treatment have been given by deGroot, Prigogine, and others.¹ The phenomenological theory of this sort is sometimes called the quasi-thermodynamical theory.

In this series of lectures I will not go into the details of quasi-thermodynamics. My subject is rather the microscopic part of the theory which we might call the statistical-mechanical theory of irreversible processes. This may well be compared to the ordinary statistical mechanics as the microscopic basis of thermodynamics. I might, however, first describe briefly the general features of quasi-thermodynamics in order to give you the background of the problems which I shall discuss in greater detail.

1.1. Simple Examples

Let us consider a few simple phenomena which may be regarded as typical showing the irreversible nature of real physical processes.

1) Two bodies, I and II, are in contact with heat baths at temperature T_I and T_{II} . The heat flows are as indicated in the figure. Heat flows from the first reservoir into I and then through the contact C of I and II to II and finally to the second reservoir. The entropy

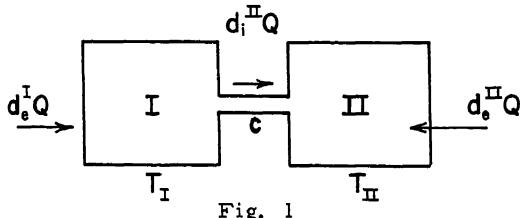


Fig. 1

* Presented at the THEORETICAL PHYSICS INSTITUTE, University of Colorado, Summer 1958

increase dS of the system I and II consists of two parts,

$$dS = d_e S + d_i S$$

$$d_e S = \frac{d_e^I Q}{T_I} + \frac{d_e^{II} Q}{T_{II}} \quad (1.1)$$

$$d_i S = d_i^I Q \left(\frac{1}{T_{II}} - \frac{1}{T_I} \right) .$$

We now assume that each body I or II is always internally at equilibrium in spite of the fact that I and II are not mutually in equilibrium. The first part $d_e S$ is the entropy change due to the exchange of I and II with their heat reservoirs, and so it may be regarded as the entropy flow coming from the outside of the system. The second part, $d_i S$, is the increase of entropy inside the system and is called the entropy production. Thermodynamically this must be positive

$$d_i S > 0 \quad (1.2)$$

because the heat transfer inside the system should always increase the entropy.

The rate of entropy change is

$$\frac{dS}{dt} = \frac{d_e S}{dt} + \frac{d_i S}{dt} .$$

In a stationary state in which heat is flowing from the hot reservoir to the cold one, we have

$$\frac{dS}{dt} = 0 \quad \frac{d_i S}{dt} > 0 \quad \frac{d_e S}{dt} < 0 .$$

The heat flow is now defined by

$$J = \frac{d_i^{II} Q}{dt} \quad (1.3)$$

and the driving force X is defined by

$$X = \frac{1}{T_{II}} - \frac{1}{T_I} \quad (1.4)$$

The relation between J and X depends on the physical situation, but we generally know that J and X vanish together and that a linear relation exists between these two quantities in so far as X is small. Then we are speaking of a linear dissipative system and assume the relation

$$J = L X \quad (1.5)$$

which gives

$$\frac{d_i S}{dt} = L X^2 \quad (1.6)$$

The only conclusion drawn generally from this relation is that

$$L > 0 \quad (1.7)$$

because the positive entropy production is characteristic of an actual irreversible process.

2) We go a step further to generalize our simple example, and assume a mass flow present between the two bodies shown in Fig. 1. The transfer of mass $-dM_I = dM_{II}$ from I to II is accompanied with an increase of entropy. Thus we have

$$\frac{d_i S}{dt} = \frac{d_i Q}{dt} \left(\frac{1}{T_{II}} - \frac{1}{T_I} \right) - \frac{dM_{II}}{dt} \left(\frac{\mu_{II}}{T_{II}} - \frac{\mu_I}{T_I} \right) \quad (1.8)$$

for the entropy production due to the flow of heat and mass. Correspondingly, we may define forces X_U and X_M by

$$X_U = \frac{1}{T_{II}} - \frac{1}{T_I} = \Delta \left(\frac{\partial S}{\partial U} \right)_M \quad (1.9a)$$

and

$$X_M = - \left(\frac{\mu_{II}}{T_{II}} - \frac{\mu_I}{T_I} \right) = \Delta \left(\frac{\partial S}{\partial M} \right)_U \quad (1.9b)$$

μ being the chemical potential. The flows are defined by

$$J_u = \frac{d_i Q}{dt} \quad J_M = \frac{d M}{dt} . \quad (1.10)$$

Obviously, equilibrium exists when $X_u = X_M = 0$. If the deviation is small from equilibrium, we may assume the linear relations

$$J_M = L_{11} X_M + L_{12} X_u \quad (1.11)$$

$$J_u = L_{21} X_M + L_{22} X_u .$$

This assumption leads us to the entropy production.

$$\frac{d_i S}{dt} = L_{11} X_M^2 + L_{12} X_u X_M + L_{21} X_u X_M + L_{22} X_u^2 \quad (1.12)$$

The positive definiteness of $d_i S/dt$ simply gives the conditions

$$L_{11} > 0 \quad L_{22} > 0 \quad (1.13)$$

$$L_{11} L_{22} - L_{12} L_{21} > 0 .$$

However, quasi-thermodynamics would not help us much if the above is all that we know about these phenomenological coefficients. It is very important to notice here the presence of a general law, ² which we call the Onsager relations, that is

$$L_{12} = L_{21} . \quad (1.14)$$

This theorem is the keystone of quasi-thermodynamics as we shall see by the following example.

We choose now T and p for the independent variables which we control. Then

$$X_u = - \frac{\Delta T}{T} \quad (1.15)$$

$$X_M = - \Delta \left(\frac{U}{T} \right) = - \frac{v \Delta P}{T} + \frac{h \Delta T}{T^2}$$

v being the specific volume and h the specific enthalpy. Equations (1.11) now take the form

$$J_M = - \frac{L_{11}v}{T} \Delta P + \frac{L_{11}h - L_{12}}{T^2} \Delta T \quad (1.16)$$

$$J_U = - \frac{L_{21}v}{T} \Delta P + \frac{L_{21}h - L_{12}}{T^2} \Delta T.$$

When $\Delta T = 0$, and $\Delta P \neq 0$, the energy flow is induced by the mass flow with the energy of transfer u^* , which is easily seen to be

$$\frac{J_U}{J_M} = \frac{L_{21}}{L_{11}} = u^* \quad (1.17)$$

A very interesting phenomenon called thermo-osmosis follows from Eq. (1.16). This is the pressure difference produced by the presence of heat flow when the mass flow is inhibited. Namely

$$\begin{aligned} \frac{\Delta P}{\Delta T} &= \frac{L_{11}h - L_{12}}{L_{11}vT} = \frac{h - L_{12}/L_{11}}{vT} = \frac{h - u^*}{vT} \\ \therefore \frac{\Delta P}{\Delta T} &= - \frac{q^*}{vT} \end{aligned} \quad (1.18)$$

This is very much like the Clausius-Clapeyron equation, but is actually another thing. The heat of transfer, q^* , is defined by

$$q^* = u^* - h \quad (1.19)$$

For a Knudsen gas in a box with a thin wall inside, the energy of transfer is calculated as

$$\begin{aligned} u^* &= \frac{\int d\mathbf{v}_x \int d\mathbf{v}_y \int d\mathbf{v}_z \frac{m}{2} v^2 \cdot n v_x f(v)}{\int d\mathbf{v}_x \int d\mathbf{v}_y \int d\mathbf{v}_z n v_x f(v)} \\ &= 2kT \end{aligned} \quad (1.20)$$

where n is the number density of molecules and $f(v)$ the Maxwell-Boltzmann distribution function. Per unit mass we may write

$$u^* = \frac{2RT}{M}$$

M being the molecular weight. The heat of transfer is now

$$q^* = U^* - h = \frac{2RT}{M} - \frac{5RT}{2M} = -\frac{RT}{2M} = -\frac{1}{2} P V$$

Thus we have

$$\frac{\Delta P}{\Delta T} = \frac{P}{2T} \quad (1.21)$$

and therefore

$$\frac{P_I}{\sqrt{T_I}} = \frac{P_{II}}{\sqrt{T_{II}}} \quad (1.22)$$

which determines the pressure difference of a Knudsen gas in the thermo-osmosis phenomena.*

Problem 1. For an ordinary dense gas, in which the mean path is short, we should have $q^* = 0$ and no thermo-osmosis phenomena. Why?

Problem 2. Discuss the thermo-mechanical (fountain) effect of liquid He II.

1.2. General Scheme of Quasi-Thermodynamical Theory

The simple example based on Eq. (1.11) may be enough to illustrate the general features of quasi-thermodynamics. We here summarize in a general way the scheme of this theory. Consider a system the macroscopic state of which is characterized by the set of macroscopic variables $\alpha_1, \alpha_2, \dots, \alpha_n$.

- 1) Flow: Generally the flows are defined by the time rate of the changes of these variables

$$\dot{J}_i = \dot{\alpha}_i \quad (1.23)$$

- 2) Force: The internal equilibrium of the system is defined by the maximum of entropy. Deviations from this maximum give rise to flows. Therefore, we may regard

$$\dot{X}_i = \frac{\partial S}{\partial \dot{\alpha}_i} \quad (1.24)$$

* Eq. (1.22) is also easily proved by simple gas kinetic theory. The integration of Eq. (1.21) to (1.22) is, however, not quite right, because (1.21) applies primarily to small difference ΔP or ΔT . Therefore, in fact, we need further justification in the reasoning here stated.

as the force conjugate to the flow J_i . The entropy S is here conceived as a function of the variables a_1, \dots, a_n . In order to make this possible, we have to assume a local equilibrium for the state defined by a given value of a 's.

- 3) Entropy production: We may take $a_1 = a_2 = \dots = a_n = 0$ to define the true equilibrium where no flow is present. Then the entropy S may be written as

$$S = S_0 + \Delta S(a_1, \dots, a_n)$$

so that the internal change of entropy, or the entropy production, is

$$\begin{aligned} \frac{d_i S}{dt} &= \frac{d \Delta S}{dt} = \sum \frac{\partial \Delta S(a)}{\partial a_i} \dot{a}_i = \sum X_i \dot{a}_i \\ &= \sum J_i X_i . \end{aligned} \quad (1.25)$$

This is a bilinear form in the flows and forces. The first axiom of quasi-thermodynamics is that

$$\frac{d_i S}{dt} = \sum J_i X_i > 0. \quad (1.26)$$

- 4) Linear relations: We confine ourselves in the linear-dissipative systems which assume the presence of the linear relations.

$$J_i = \sum_k L_{ik} X_k \quad (1.27)$$

between the flows and the forces. The L 's here are called the kinetic coefficients.

- 5) Onsager relations:² Considering the problem of heat conduction in anisotropic crystals, Onsager established a very general theorem, which we now call the Onsager relations. This theorem states the reciprocity law:

$$L_{ik}(\vec{H}) = L_{ki}(-\vec{H}) \quad (1.28)$$

$$L_{ik}(\vec{\omega}) = L_{ki}(-\vec{\omega})$$

where \vec{H} is the magnetic field and $\vec{\omega}$ represents the vector of

angular velocity. \vec{H} and $\vec{\omega}$ must be reversed to preserve the reciprocity if the system we observe is actually in a magnetic field or is rotating.

Quasi-thermodynamics as a phenomenological theory cannot say anything about the phenomenological coefficients. It would be almost useless if we did not know the Onsager relations. Thanks to the Onsager relations, quasi-thermodynamics can establish some general statements and can correlate different phenomena in a general way. The role of quasi-thermodynamics, even though not as powerful, resembles that of thermodynamics.

1.3. The Onsager Relations

We shall briefly describe the original proof of the Onsager relations.² When we talk about an irreversible process which consists in the time change of the variables $\alpha_1, \dots, \alpha_n$, we take these variables as controllable at least in principle. Thus, we shift these variables from their equilibrium values and produce a certain flow, which is phenomenologically described by such equations as (1.27), or

$$\dot{\alpha}_j = \sum_k L_{jk} \frac{\partial \Delta S}{\partial \alpha_k}, \quad (1.29)$$

Now Onsager assumed that the same law (1.29) should hold for the average regression of fluctuations which may take place in the neighborhood of the equilibrium.

For instance, two bodies in thermal contact may have a temperature difference ΔT as the result of thermal fluctuation at a certain time t . Knowing this fact, $\Delta T(t + \tau)$ may be expected to be finite on the average, but it will on the average decrease as τ grows. Onsager assumed that this decrease on the average follows the macroscopic law of heat conduction. To make the statement clearer, we define

$$\alpha_j(t + \tau | t, \alpha') \quad (1.30)$$

as a random variable to represent the observed value of α_j at the time $t + \tau$ when the values of α_k ($k = 1, \dots, n$) at the time t were known to be

$$\alpha_k = \alpha'_k, \quad k = 1, \dots, n.$$

We talk about random variables because the observed values of the quantities α 's are statistical in nature. Prescription of the α 's can by no means fix the microscopic state of our system. We further have to assume the statistical law which is obeyed by our system. We assume our system to be an aged one. This means that an internal equilibrium is

attained in our system which has been left alone for a long time. Fluctuations occurring in the system are ergodic in the sense of the word as used in the probability theory of stationary time series. Now Onsager's assumption may be expressed as

$$\frac{1}{\tau} \overline{\{d_j(t+\tau|t, d') - d'_j\}} = \sum_k L_{jk} X_k(d') . \quad (1.31)$$

The left-hand side is the time rate of the change of the expectation value of d_j over the interval τ . The right-hand side is the force at the time t . It should be noticed that the interval τ must neither be too short nor too long. It should be short on macroscopic scale in order that the left-hand side be replaced by a time derivative corresponding to Eq. (1.29). It should be long on microscopic scale in order that we have a macroscopic law. Taking an average over the distribution of the initial states specified by $\{d'_j\}$ in Eq. (1.31), we get

$$\frac{1}{\tau} \langle \overline{\{d_j(t+\tau|t, d') - d'_j\}} d'_l \rangle = \sum_m L_{jm} \langle X_m(d') d'_l \rangle \quad (1.32)$$

where $\langle \cdot \rangle$ means an average over the statistical ensemble with the distribution function

$$P(d') = C e^{\Delta S(d')/k} \quad (1.33)$$

The left hand side of the above equation may be simply written as

$$\frac{1}{\tau} \langle d_j(t+\tau) d'_l(t) - d_j(t) d'_l(t) \rangle$$

where $d_j(t)$ means the value of d_j at time t induced by the internal motion of the system. The right-hand side is easily transformed to

$$\begin{aligned} \langle X_m(d') d'_l \rangle &= \left\langle \frac{\partial \Delta S(d')}{\partial d'_m} d'_l \right\rangle \\ &= \int \cdots \int P(d') dd' \frac{\partial S(d')}{\partial d'_m} d'_l \\ &= C \int \cdots \int e^{\Delta S(d')/k} dd' \frac{\partial \Delta S(d')}{\partial d'_m} d'_l \\ &= kC \int \cdots \int \frac{\partial}{\partial d'_m} \left(e^{\Delta S(d')/k} \right) \cdot d'_l dd' \cdots dd_n \end{aligned}$$

$$= -k \delta_{jm}$$

Therefore, Eq. (1.32) now gives

$$\frac{1}{\tau} \langle \{\alpha_j(t+\tau) - \alpha_j(t)\} \alpha_l(t) \rangle = -k L_{jl} \quad (1.34)$$

which may as well be written as

$$\frac{1}{\tau} \langle \{\alpha_j(\tau) - \alpha_j(0)\} \alpha_l(0) \rangle = -k L_{jl} \quad (1.34a)$$

because the system in consideration is aged and thus stationary. Eq. (1.34) may be seen as an expression of the kinetic coefficient from which we see easily that the Onsager relations (1.28) must hold. All we have to show is that the relation

$$\langle \alpha_j(t) \alpha_l(0) \rangle_{\vec{H}} = \langle \alpha_l(t) \alpha_j(0) \rangle_{-\vec{H}} \quad (1.35)$$

holds in the presence of the magnetic field \vec{H} . * The classical equations of motion are given by

$$\dot{P} = -\frac{\partial H}{\partial q}, \quad \dot{q} = \frac{\partial H}{\partial P} \quad (1.36)$$

where p and q represent all sets of canonical variables. One solution of the equation (1.36) will be designated by $\{P(t), q(t)\}$. We define a solution reciprocal to this by

$$\begin{aligned} P^*(t) &= -P(-t) \\ q^*(t) &= q(-t). \end{aligned} \quad (1.37)$$

Since

$$\frac{dP^*(t)}{dt} = \dot{P}(-t) = -\frac{\partial H}{\partial q} \Big|_{t \rightarrow -t} = -\frac{\partial H(-P^*, q^*)}{\partial q^*}$$

* A similar proof can easily be made for a rotating system, which is left for readers as an exercise. In the following also we shall talk about magnetic field rather than rotation, mainly for reasons of physical interest.

and

$$\frac{d q^*(t)}{dt} = -\dot{q}(t) = -\left. \frac{\partial H}{\partial P} \right|_{t \rightarrow -t} = -\frac{\partial H(-P^*, q^*)}{\partial (-P^*)}$$

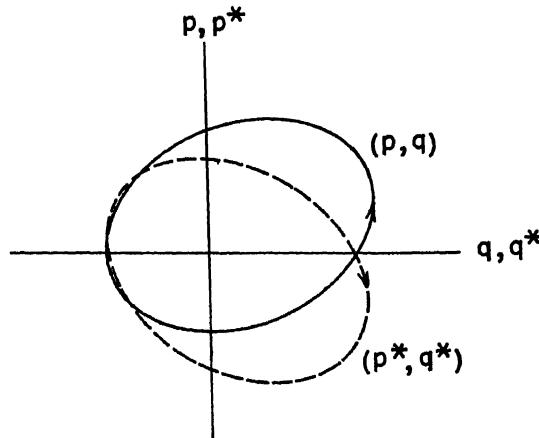


Fig. 2

the reciprocal motion $\{p^*(t), q^*(t)\}$ is a solution of the canonical equations

$$\frac{d P^*(t)}{dt} = -\frac{\partial H^*}{\partial q^*}, \quad \frac{d q^*(t)}{dt} = \frac{\partial H^*}{\partial P^*} \quad (1.38)$$

which describes a dynamical system with the Hamiltonian

$$H^*(P^*, q^*) = H(-P^*, q^*) \quad (1.39)$$

Now Eq. (1.35) is proved as follows. We write

$$\langle d_j(t) d_l(0) \rangle_H \quad (1.40)$$

$$= \int f_H(P_0, q_0) d_j(P_t, q_t) d_l(P_0, q_0) d\Gamma_0$$

where (P_0, q_0) stands for the initial point in the phase space, the volume element for which is here denoted by $d\Gamma_0$, and (q_t, P_t) represents the motion of the phase point starting from (P_0, q_0) at $t = 0$ following the equation of motion (1.36). $f_{\vec{H}}(P_0, q_0)$ is the distribution function in the phase space, \vec{H} being the magnetic field applied to the system. Since f represents the equilibrium distribution, we ought to have

$$f_{\vec{H}}(P_0, q_0) d\Gamma_0 = f_{\vec{H}}(P_t, q_t) d\Gamma_t \quad (1.41)$$

for any t . Thus, Eq. (1.40) is transformed as follows:

$$\begin{aligned} & \langle \phi_j(t) \phi_\ell(0) \rangle_{\vec{H}} \\ &= \int f_{\vec{H}}(P_0, q_0) \phi_j(P_0, q_0) \phi_\ell(P_{-t}, q_{-t}) d\Gamma_0 \\ &= \int f_{\vec{H}}(-P_0^*, q_0^*) \phi_j(-P_0^*, q_0^*) \phi_\ell(-P_t^*, q_t^*) d\Gamma^* \quad (1.42) \\ &= \int f_{-\vec{H}}(P_0^*, q_0^*) \epsilon_j \phi_j(P_0^*, q_0^*) \epsilon_\ell \phi_\ell(P_t^*, q_t^*) d\Gamma^* \\ &= \epsilon_j \epsilon_\ell \langle \phi_\ell(t) \phi_j(0) \rangle_{-\vec{H}} \end{aligned}$$

because the Hamiltonian changes as

$$H_{\vec{H}}(P, q) = H_{-\vec{H}}(-P, q)$$

by the change of direction of magnetic field, so that the distribution function $f_{\vec{H}}(-P_0^*, q_0^*)$ is equal to $f_{-\vec{H}}(P_0^*, q_0^*)$. ϵ_j in Eq. (1.42) is equal to +1 or -1 according to ϕ_j be even or odd in the momenta p . Therefore, we have now proved the Onsager reciprocity law.

$$L_{j\ell}(\vec{H}) = \epsilon_j \epsilon_\ell L_{\ell j}(-\vec{H}). \quad (1.43)$$

In most cases ϵ_j and ϵ_ℓ have the same sign so that (1.43) reduces to (1.28).

1.4 Other Derivations of the Onsager Relations

Takahashi³ gave an elegant theory of thermal fluctuation for a classical system, which will be briefly summarized. He starts from a

general law of statistical mechanics which defines a statistical average $\langle u \rangle$ by

$$\langle u \rangle = \int dP u e^{-H/kT} / \int dP e^{-H/kT} \quad (1.44)$$

for any quantity u . Now suppose the Hamiltonian H involves a parameter x so that u itself and $\langle u \rangle$ depend on x . One obtains easily

$$\langle ux \rangle - \langle u \rangle \langle x \rangle = kT \left\{ \frac{\partial \langle u \rangle}{\partial x} - \langle \frac{\partial u}{\partial x} \rangle \right\} \quad (1.45)$$

by differentiating (1.44) by x , where X is defined by

$$X = - \frac{\partial H}{\partial x} \quad (1.46)$$

Since u in this equation is arbitrary, we may choose it as

$$u(P_\tau) \equiv u^\tau(P)$$

where P represents a phase point and P_τ is the phase point at the time τ which was located at P at the time $\tau=0$. u^τ simply describes the change of u induced by the motion. Thus, we have

$$\langle u^\tau X \rangle - \langle u^\tau \rangle \langle X \rangle = kT \left\{ \frac{\partial \langle u^\tau \rangle}{\partial x} - \langle \frac{\partial u^\tau}{\partial x} \rangle \right\} \quad (1.47)$$

On the right-hand side $\langle u^\tau \rangle$ may be written as $\langle u \rangle$ since the system is in equilibrium, so that

$$\frac{\partial \langle u^\tau \rangle}{\partial x} \delta X = \frac{\partial \langle u \rangle}{\partial x} \delta X$$

represents the response of u when the parameter x is changed by δx keeping the temperature constant at T , whereas

$$\langle \frac{\partial u^\tau}{\partial x} \rangle \delta X = \langle \delta u^\tau \rangle \quad (1.48)$$

means the average change of u at the time τ when a sudden change δx is given at $\tau=0$ (see Fig. 3). Therefore, we may write

$$\langle \frac{\partial u^\tau}{\partial x} \rangle = \sum_e e \langle \tau \rangle \quad (1.49)$$

and may call Φ^e the after effect function. We may put also,

$$\frac{\partial \langle u \rangle}{\partial x} = \Phi^e(\infty) \quad (1.50)$$

if the system should attain an equilibrium after lapse of an infinite time without appreciable change of the temperature. This is not always true, but is true in such practical cases where the heat capacity of those degrees of freedom not directly associated with x is large compared to that associated with x . Assuming this, Eq. (1.47) may be written as

$$\langle (u^\tau - \langle u \rangle)(x - \langle x \rangle) \rangle = kT \{ \Phi^e(\infty) - \Phi^e(\tau) \} = kT \Phi(\tau) \quad (1.51)$$

where the function $\Phi(\tau)$ may be called the relaxation function. (See Fig. 3.)

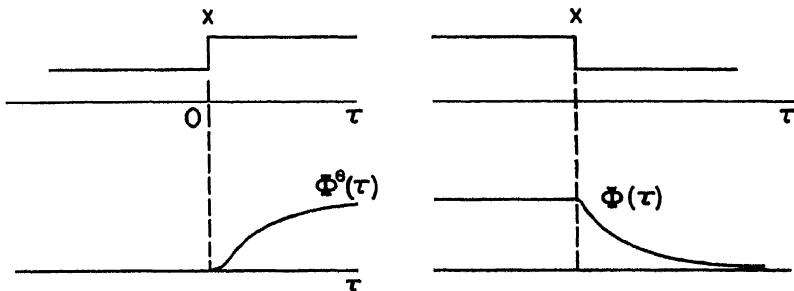


Fig. 3

Eq. (1.51) represents a general law which connects the time correlation of thermal fluctuations occurring spontaneously in equilibrium with the after effect function or the relaxation function which describes the response of the system when we exert actively a disturbance from outside to change the parameter x . This replaces Onsager's assumption of the applicability of macroscopic laws to the average regression of spontaneous fluctuation.

Let now $\{X_j\}$ be a set of parameters which are controlled. Taking x and u as X_j and X_{j+1} in Eq. (1.51) we have

$$\langle (X_j^\tau - \langle X_j \rangle)(X_{j+1} - \langle X_{j+1} \rangle) \rangle = kT \Phi_{j,j+1}(\tau) \quad (1.52)$$

for the relaxation function $\Phi_{j,j+1}(\tau)$ which describes the relaxation of X_{j+1} after removal of a strain δX_j . Instead of (1.52) we may write

$$\langle (x_l^r - x_l) x_j \rangle = kT \Phi_{lj}^e (\tau)$$

$$= kT \left\langle \frac{\delta x_l(t+\tau)}{\delta x_j(t)} \right\rangle$$

where $\delta x_l(t+\tau)/\delta x_j(t)$ is a functional derivative to give the effect of a change $\delta x_j(t)$ at time t on x_l at $t + \tau$. The reciprocity law is expressed as

$$\left\langle \frac{\delta x_l(t+\tau)}{\delta x_j(t)} \right\rangle_H = E_j E_l \left\langle \frac{\delta x_j(t+\tau)}{\delta x_l(t)} \right\rangle_{-H} \quad (1.53)$$

as one sees easily from Eq. (1.42). The reciprocity law in this form is more general than that of Onsager and includes the latter.

Problem 3. Suppose that the possible states of the system are the set $\{\lambda\}$ and the dynamical motion of the system is in some ways approximated by a Markoffian process

$$\dot{P}_{\lambda\mu}(t) = - \sum_{\nu} P_{\lambda\nu}(t) \Lambda_{\nu\mu} + \sum_{\nu} P_{\lambda\nu}(t) \Lambda_{\mu\nu}$$

where $P_{\lambda\mu}(t)$ is the probability for finding the system in the state μ at the time t knowing that it was in λ at $t = 0$ and $\Lambda_{\nu\mu}$ is the transition probability. Replacing the left-hand side of Eq. (1.34) by a time-derivative, shows, that the kinetic coefficient L_{jj} is expressed as

$$L_{jj} = \frac{1}{2k} \sum_{\lambda} \sum_{\mu} (d_{j\lambda} - d_{j\mu})(d_{j\lambda} - d_{j\mu}) \Lambda_{\lambda\mu} / \bar{w}$$

where $d_{j\lambda}$ is the value of the quantity d_j in the state λ and \bar{w} is the total number of possible states. Magnetic field or rotation is assumed not to exist for simplicity.⁴

II. Linear Dissipative Systems

In part I, we saw that the phenomenological coefficients of the quasi-thermodynamical theory are actually related to fluctuation processes taking place in the system at equilibrium. We shall now pursue further this line of consideration and examine more in detail what it implies.⁵

2.1. Response to a Dynamical Disturbance

We consider the response of the system to a change of forces which are controlled by us. Let us assume that the force is of a dynamical

nature and may be represented by an additional term H_{ext} of the Hamiltonian, i. e.,

$$H_t = H_{ext} + H, \quad H_{ext} = -AF(t) \quad (2.1)$$

where F is a force and H is the unperturbed Hamiltonian.

First we shall discuss the classical case, where the system in question is statistically represented by a distribution function which follows the equation of motion

$$\frac{\partial f_t}{\partial t} = - \sum \left(\frac{\partial f_t}{\partial q} \frac{\partial H_t}{\partial p} - \frac{\partial f_t}{\partial p} \frac{\partial H_t}{\partial q} \right) \equiv (H_t, f_t), \quad (2.2)$$

where the bracket means the Poisson bracket, i. e.,

$$(A, B) = \sum \left(\frac{\partial A}{\partial q} \frac{\partial B}{\partial p} - \frac{\partial A}{\partial p} \frac{\partial B}{\partial q} \right)$$

Assuming that the outer disturbance is small, we express the distribution function by an unperturbed part plus a small perturbation function

$$f_t = f + \Delta f \quad (2.3)$$

where f is the equilibrium distribution function satisfying the condition

$$(H, f) = 0 \quad (2.4)$$

Inserting (2.1) and (2.3), Eq. (2.2) gives

$$\frac{\partial \Delta f}{\partial t} = (H, \Delta f) - F(t)(A, f), \quad (2.5)$$

which determines Δf in the first order of perturbation. Eq. (2.5) may conveniently be written as

$$\frac{\partial \Delta f}{\partial t} = iL \Delta f - F(t)(A, f) \quad (2.6)$$

in order to indicate the fact that the Poisson bracket operation is a linear operation, e. g.

$$iLg \equiv (H, g) \quad (2.7)$$

It should be remembered that $\exp(iLt)$ represents the unperturbed or natural motion of the system. It induces the natural motion of a phase point P to P_t over the time t , or symbolically,

$$\mathcal{L}^{-itL} P_0 = P_t \quad (2.8)$$

Correspondingly, the natural motion of any dynamical quantity $A(p, q) \equiv A(p)$ is given by

$$A(t) \equiv A(P_t) = \mathcal{L}^{-it\tau L} A(P_{t-\tau})$$

which is the solution of the equation of motion

$$\frac{dA}{dt} = (A, H)$$

This corresponds to the Heisenberg picture in quantum mechanics.

The inhomogeneous Eq. (2.6) can easily be solved to give

$$\Delta f(t) = - \int_{-\infty}^t \mathcal{L}^{i(t-t')L} (A, f) dt' \cdot F(t') \quad (2.9)$$

since we assumed $F(-\infty) = 0$, $\Delta F(-\infty) = 0$. That is, the system was assumed to be in equilibrium at $t = -\infty$.

Now the expectation value of an arbitrary quantity B is given by

$$\begin{aligned} \langle \Delta B(t) \rangle &= \int B \Delta f(t) d\Gamma \\ &= - \int_{-\infty}^t dt' \int d\Gamma B e^{i(t-t')L} (A, f) F(t') \\ &= - \int_{-\infty}^t dt' F(t') \int (A, f) B(t-t') d\Gamma \end{aligned}$$

This may be written as

$$\langle \Delta B(t) \rangle = \int_{-\infty}^t \phi_{BA}(t-t') F(t') dt' \quad (2.10)$$

where*

$$\begin{aligned}\phi_{BA}(t) &= \int (f, A) B(t) d\Gamma & (2.11) \\ &= \int f(A, B(t)) d\Gamma\end{aligned}$$

is defined as the response function which describes the response of the system showing up in B by application of a pulse (see Fig. 4).

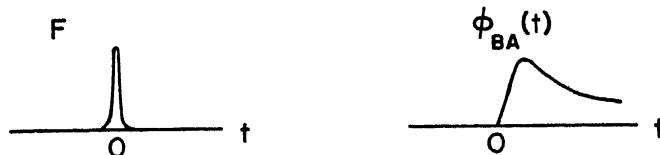


Fig. 4

Eq. (2.11) can be interpreted as follows. $-(A, f)$ is the change of the distribution function produced by a pulse. The effect of this on the average value of B at a later time is given by the first equation of (2.11). Instead of talking about the change of distribution function, we may also think of the effect of the pulse on the motion of B. In the last equation of (2.11), $(A, B(t))$ represents such an effect.

If the distribution f is assumed to be canonical

$$f = C e^{-\beta H}, \quad \beta = \frac{1}{kT}$$

we evidently have

$$(f, A) = \beta \dot{A} f,$$

*

$$\begin{aligned}\int d\Gamma B e^{i\tau L} (A, f) &= \int d\Gamma_{P_0} B(P_0) (A, f) (P_0) \\ &= \int d\Gamma_{P_t} B(P_t) (A, f) (P_0) \\ &= \int d\Gamma_{P_t} B(P_t) (A, f) (P_0) \quad (\because d\Gamma_{P_t} = d\Gamma_{P_0})\end{aligned}$$

so that Eq. (2.11) may be expressed as

$$\phi_{BA}(t) = \beta \langle \dot{A}(0) B(t) \rangle = -\beta \langle A(0) \dot{B}(t) \rangle, \quad (2.12)$$

where we used the stationary condition

$$\frac{d}{dt} \langle A(t), B(t+\tau) \rangle = 0$$

2.2. Quantum-Mechanical Treatment

It is easy to revise the foregoing classical theory into a quantum-mechanical form. The distribution function is replaced by the density matrix ρ , the Poisson bracket by commutator operation, and the phase integration by the trace operation. Thus, Eq. (2.5) now goes into

$$\frac{\partial \Delta \rho}{\partial t} = \frac{1}{i\hbar} [\mathcal{H}, \Delta \rho] - \frac{1}{i\hbar} [A, \rho] F(t) \quad (2.13)$$

It is very convenient to introduce a linear operator \mathcal{H}^* by the definition

$$\mathcal{H}^* G \equiv [\mathcal{H}, G]$$

\mathcal{H}^* is an operator which operates upon other operators.* By this definition the solution of Eq. (2.13) is written as

$$\Delta \rho = - \int_{-\infty}^t e^{(t-t')\mathcal{H}^*/i\hbar} \frac{1}{i\hbar} [A, \rho] \cdot F(t') dt' \quad (2.14)$$

* The commutator operation a^* follows the rules:

$$a^* b - b a^* = [a, b]^* \quad \therefore [a, [b, c]] - [b, [a, c]] = [[a, b], c]$$

$$e^{a^*} b = e^a b e^{-a}$$

$$e^{a^*} b = \sum \frac{1}{n!} (a^*)^n b$$

$$= \sum \frac{1}{n!} [a \overbrace{[a \dots [a}^n b] \dots]$$

$$= e^a b e^{-a}$$

in parallel to Eq. (2.8). Thus we have

$$\begin{aligned}\overline{\Delta B(t)} &= \text{Tr} \Delta \rho(t) B \\ &= \frac{1}{i\hbar} \int_0^t \text{Tr} [A, \rho] B(t-t') F(t') dt'\end{aligned}\quad (2.15)$$

where

$$B(t) = e^{itH/\hbar} B e^{-itH/\hbar}$$

is a Heisenberg operator. The response function (2.11) is now

$$\begin{aligned}\phi_{BA}(t) &= \frac{1}{i\hbar} \text{Tr} [\rho, A] B(t) \\ &= \frac{1}{i\hbar} \text{Tr} \rho [A, B(t)]\end{aligned}\quad (2.16)$$

which is just a quantal version of (2.11). If ρ is assumed to be canonical, we make use of the identity

$$\begin{aligned}[\rho, A] &\equiv \int_0^\beta e^{\lambda H} [A, H] e^{-\lambda H} d\lambda \\ &= i\hbar \int_0^\beta \dot{\rho} A(-i\hbar\lambda) d\lambda\end{aligned}\quad (2.17)$$

and rewrite Eq. (2.16) as

$$\begin{aligned}\phi_{BA}(t) &= \int_0^\beta d\lambda \text{Tr} [\rho \dot{A}(-i\hbar\lambda) B(t)] \\ &= - \int_0^\beta d\lambda \text{Tr} [\rho A(-i\hbar\lambda) \dot{B}(t)]\end{aligned}\quad (2.18)$$

which corresponds to Eq. (2.12).

A serious question may be raised about this treatment pointing out how we know that the calculated average $\langle B(t) \rangle$ actually represents what is observed by experiments. This question involves two things. The first is the average over an ensemble. This is quite the same as that which we have in ordinary statistical mechanics. We observe only one system, but the observed value is identified with the statistical average over an ensemble of similar systems. This is justified by the nature of the quantity, B , and of the system in question which are both really macroscopic. The

second is concerned with the disturbances which may arise from the observation process. By Eq. (2.15) we calculated an ensemble average of $\Delta B(t)$, each member of the ensemble being allowed to continue its own course without suffering any disturbance by observation. Actually, we are observing the response of a single system by some means, so that the system may be continuously disturbed. This is not taken into account in the calculation of (2.15). We just do not know at present how to answer this difficult question. An optimist may anticipate that such a quantum-mechanical disturbance is not important for such quantities we may deal with and for such kind of observation processes.⁶

2.3. General Expressions of Admittance and Symmetry Relations

We now apply Eq. (2.10) to a periodic disturbance,

$$\begin{aligned} F(t) &= F_0 e^{i\omega t} \\ &= \lim_{\epsilon \rightarrow 0^+} F_0 e^{i\omega t + \epsilon t} \end{aligned} \quad (2.19)$$

We write the second expression in order to show that the disturbance has been switched on adiabatically in the infinite past. For a periodic disturbance, the response may be expressed as

$$\langle \Delta B(t) \rangle = R_e \chi_{BA}(\omega) F_0 e^{i\omega t} \quad (2.20)$$

where $\chi_{BA}(\omega)$ is the complex susceptibility, which is now simply a Fourier-transform of the response function,

$$\begin{aligned} \chi_{BA}(\omega) &= \int_0^\infty \phi_{BA}(t) e^{-i\omega t} dt \\ &= \lim_{\epsilon \rightarrow 0^+} \int_0^\infty \phi_{BA}(t) e^{-i\omega t - \epsilon t} dt \end{aligned} \quad (2.21)$$

The latter relation is obtained by one's inserting (2.19) into (2.10). Eq. (2.21) may be written in other ways,

$$\begin{aligned} \chi_{BA}(\omega) &= \lim_{\epsilon \rightarrow 0^+} \frac{1}{i\omega + \epsilon} \left\{ \phi_{BA}(0) + \int_0^\infty \phi_{BA}(t) e^{-i\omega t - \epsilon t} dt \right\} \\ &= \Phi_{BA}(0) - i\omega \int_0^\infty \Phi_{BA}(t) e^{-i\omega t} dt \end{aligned} \quad (2.22)$$

by partial integration. $\Phi_{BA}(t)$ here is defined by

$$\Phi_{BA}(t) = \int_t^{\infty} \phi_{BA}(t') dt' \quad (2.23)$$

which is called the relaxation function describing the relaxation. (See Fig. 3.)

By Eqs. (2.12) and (2.18), (2.23) may be integrated to give

$$\Phi_{BA}(t) = \beta \langle AB(t) - A^o B^o \rangle \quad (\text{classical}) \quad (2.24)$$

$$= \int_0^{\beta} d\lambda \text{Tr} [PA(-i\hbar\lambda)B(t)] - \beta \text{Tr} \rho A^o B^o \quad (\text{quantal}) \quad (2.25)$$

where A^o or B^o means the invariant part of A or B with respect to the natural motion. The quantity A^o is defined by

$$\begin{aligned} A^o &= \lim_{s \rightarrow 0^+} s \int_0^{\infty} e^{-st} A(t) dt \\ &= \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T A(t) dt \end{aligned} \quad (2.26)$$

so that it is equal to the time average. Therefore, $\Phi_{BA}(t)$ as defined by (2.24) and (2.25) has the property that there remains no constant part as $t \rightarrow \infty$. In fact, it goes to zero as $t \rightarrow \infty$, or it simply oscillates. This may be written as

$$\Phi(t) \sim 0 \quad \text{as } t \rightarrow \infty \quad (2.27)$$

in the generalized sense of limit.

The symmetry of the functions $\Phi_{BA}(t)$ and $\chi_{BA}(\omega)$ can easily be seen.* Since the classical symmetry of $\Phi_{BA}(t)$ was already discussed, we shall examine the quantal case.

The relaxation function $\Phi_{BA}(t)$ has the following properties.

1. $\Phi_{BA}(t)$ is real
2. $\Phi_{BA}(-t) = \Phi_{AB}(t)$
3. $\Phi_{BA}(t, \vec{H}) = \xi_A \xi_B \Phi_{BA}(-t, -\vec{H})$
 $= \xi_A \xi_B \Phi_{AB}(t, -\vec{H})$

* The symmetry of the admittance was discussed generally by Casimir.⁷

These relations will be proved for the function

$$\bar{\Phi}'_{BA}(t) = \int_0^{\beta} d\lambda \operatorname{Tr} \rho A(-i\hbar\lambda) B(t) \quad (2.29)$$

because the last term (2.25) has evidently the same symmetry as $\bar{\Phi}'_{BA}(t)$.

$$\begin{aligned} 1. \quad & \overline{\bar{\Phi}'_{BA}(t)} = \int_0^{\beta} \overline{\operatorname{Tr} \rho B(t) A(i\hbar\lambda)} d\lambda = \int_0^{\beta} \overline{\operatorname{Tr} \rho B(t-i\hbar\lambda)} A d\lambda \\ & = \int_0^{\beta} \overline{\operatorname{Tr} \rho B(t-i\hbar(\beta-\lambda))} A d\lambda = \int_0^{\beta} \overline{\operatorname{Tr} \rho A B(t+i\hbar\lambda)} d\lambda = \bar{\Phi}'_{BA}(t) \\ 2. \quad & \bar{\Phi}'_{BA}(t) = \int_0^{\beta} \overline{\operatorname{Tr} \rho A B(t+i\hbar\lambda)} d\lambda = \int_0^{\beta} \overline{\operatorname{Tr} \rho A(t-i\hbar\lambda)} B d\lambda \\ & = \int_0^{\beta} \overline{\operatorname{Tr} \rho B A(t+i\hbar\lambda)} d\lambda = \bar{\Phi}'_{AB}(t) \end{aligned}$$

3. Time reversal with reverse of magnetic field changes the wave function to its conjugate. This results in

$$\epsilon_A \epsilon_B \overline{\bar{\Phi}'_{BA}(-t, -\vec{H})} = \bar{\Phi}'_{BA}(t, \vec{H})$$

By (2.22), the above mentioned symmetry leads to the same kind of symmetry for the susceptibility. We write this conveniently for $\bar{\epsilon}_{BA}(\omega)$ defined by

$$\bar{\epsilon}_{BA}(\omega) = \int_0^{\infty} \bar{\Phi}'_{BA}(t) e^{-i\omega t} dt$$

This has the following symmetry:

1. $\operatorname{Re} \bar{\epsilon}_{BA}(\omega) = \operatorname{Re} \bar{\epsilon}_{BA}(-\omega)$
2. $\operatorname{Im} \bar{\epsilon}_{BA}(\omega) = -\operatorname{Im} \bar{\epsilon}_{BA}(-\omega)$ (2.30)
3. $\bar{\epsilon}_{BA}(\omega, -\vec{H}) = \epsilon_A \epsilon_B \bar{\epsilon}_{AB}(\omega, \vec{H})$

Consequently,

$$\begin{aligned}
 1. \operatorname{Re} \mathfrak{S}_{BA}(\omega, \vec{H}) &= \operatorname{Re} \mathfrak{S}_{BA}(-\omega, \vec{H}) = \epsilon_A \epsilon_B \operatorname{Re} \mathfrak{S}_{AB}(\omega, -\vec{H}) \\
 2. \operatorname{Im} \mathfrak{S}_{BA}(\omega, \vec{H}) &= -\operatorname{Im} \mathfrak{S}_{BA}(-\omega, \vec{H}) \\
 &= \epsilon_A \epsilon_B \operatorname{Im} \mathfrak{S}_{AB}(\omega, -\vec{H})
 \end{aligned} \quad (2.31)$$

2.4. Correlation Function

We have found that the admittance in general is simply the Fourier transform of the response function or the relaxation function (Eq. (2.21), (2.22)). As was discussed before, these functions represent the effect of a certain change in a variable on some other variable at a later time (Eq. (2.11)). In classical cases, these functions are expressed by Eqs. (2.12) and (2.24). In quantum-mechanical cases, however, the relaxation function

$$\Phi_{BA}(t) = \int_0^{\infty} d\lambda \operatorname{Tr} \rho A(-i\hbar\lambda) B(t) \quad (2.32)$$

is not itself a correlation function. The quantum-mechanical correlation function of $A(0)$ and $B(t)$, the correlation of A and B at different time points, may be defined by

$$\Psi_{BA}(t) = \operatorname{Tr} \rho \{A(0)B(t)\} \quad (2.33)$$

where $\{ \}$, the symmetrized product,

$$\{AB\} = \frac{1}{2}(AB + BA)$$

is used because $A(0)$ and $B(t)$ do not necessarily commute.

The functions $\Phi_{BA}(t)$ and $\Psi_{BA}(t)$ are shown to be mutually related by the following equations:

$$\Phi_{BA}(t) = \int_{-\infty}^{\infty} \Gamma(t-t') \Psi_{BA}(t') \quad (2.34)$$

$$\Psi_{BA}(t) = E_B \left(\frac{d}{idt} \right) \Phi_{BA}(t) \quad (2.35)$$

where $E_B(\omega)$ is the average energy of a harmonic oscillator with the frequency ω at the temperature $T = 1/k_B$ i. e.,

$$E_\beta(\omega) = \frac{\hbar\omega}{2} \coth \frac{\beta\hbar\omega}{2} \quad (2.36)$$

and the integral kernel $\Gamma(t)$ is defined by

$$\Gamma(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{e^{i\omega t}}{E_\beta(\omega)} d\omega = \frac{2}{\hbar\pi} \log \coth \frac{\pi}{2\beta\hbar} |t| \quad (2.37)$$

In the classical limit

$$\lim_{\hbar \rightarrow 0} \Gamma(t) = \beta \delta(t) \quad (2.38)$$

so that Eq. (2.34) coincides with Eq. (2.24).

In terms of the Fourier components of $\Phi_{BA}(t)$ and $\Psi_{BA}(t)$

$$f_{BA}(\omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \Phi_{BA}(t) e^{-i\omega t} dt \quad (2.39)$$

$$g_{BA}(\omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \Psi_{BA}(t) e^{-i\omega t} dt$$

Eqs. (2.34) and (2.35) are simply expressed as

$$g_{BA}(\omega) = E_\beta(\omega) f_{BA}(\omega) \quad (2.40)$$

These relations can be obtained by writing explicit forms in matrix elements and by rearranging the series. One may instead calculate in the following way:

$$\begin{aligned} f_{BA}(\omega) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} dt \int_0^\beta \text{Tr} \rho AB(t + i\hbar\lambda) e^{-i\omega t} d\lambda \\ &= \frac{1}{2\pi} \int_{-\infty}^{\infty} dt \int_0^\beta \text{Tr} \rho AB(t + i\hbar\lambda) e^{-i\omega(t+i\hbar\lambda) - \lambda\hbar\omega} d\lambda \end{aligned} \quad (2.41)$$

$$\begin{aligned}
 &= \frac{1}{2\pi} \int_0^{\beta} d\lambda e^{-i\hbar\omega \int_{-\infty+i\hbar\lambda}^{\infty+i\hbar\lambda} \text{Tr } \rho AB(t) e^{-i\omega t} dt} \\
 &= \frac{1-e^{-\beta\hbar\omega}}{\hbar\omega} \frac{1}{2\pi} \int_{-\infty}^{\infty} \text{Tr } \rho AB(t) e^{-i\omega t} dt.
 \end{aligned}$$

On the assumptions that

$$1. \lim_{\Re t \rightarrow \pm\infty} \text{Tr } \rho AB(t) = 0$$

2. $\text{Tr } \rho AB(t)$ is analytic in t in the domain $0 \leq \text{Im } t \leq \beta\hbar$

Similarly we may show that

$$\int_{-\infty}^{\infty} \text{Tr } \rho AB(t) e^{-i\omega t} dt = e^{i\hbar\omega \int_{-\infty}^{\infty} \text{Tr } \rho B(t) A(t) e^{-i\omega t} dt} \quad (2.42)$$

In this calculation ρ is taken as canonical. Eqs.(2.41) and (2.42) easily lead to (2.40). Finally we note that the symmetry of $\bar{\Psi}_{BA}(t)$ is the same as $\bar{\Phi}_{BA}(t)$.

2.5. Simple Examples

In order to illustrate the foregoing formal treatment by physical examples, we consider a magnetic problem and a conduction problem.

1. When a magnetic field $\vec{H}(t)$ is applied to a magnetic body, the perturbation is

$$H_{\text{ext}}(t) = -\vec{M} \cdot \vec{H}(t) \quad . \quad (2.43)$$

We now ask for the response in M_μ when the magnetic field is in the \sim direction. The response function for this is, by Eq. (2.16),

$$\phi_{\mu 0}(t) = \frac{1}{i\hbar} \langle [M_0, M_\mu(t)] \rangle \quad (2.44)$$

and the relaxation function is now

$$\bar{\Phi}_{\mu 0}(t) = \int_0^{\beta} \langle (M_0(-i\hbar\lambda) - M_0^\circ)(M_\mu(t) - M_\mu^\circ) \rangle d\lambda \quad . \quad (2.45)$$

The complex susceptibility $\chi_{\mu 0}(\omega)$ is, by Eq. (2.22),

$$\chi_{\mu\nu}(\omega) = \Phi_{\mu\nu}(0) - i\omega \int_0^\infty \Phi_{\mu\nu} e^{-i\omega t} dt \quad (2.46)$$

In particular, for the static magnetic field we have

$$\begin{aligned} \chi_{\mu\nu}(0) &= \Phi_{\mu\nu}(0) \\ &= \int d\lambda \langle (M_\nu (-i\hbar\lambda) - M_\nu^0)(M_\mu - M_\mu^0) \rangle \end{aligned} \quad (2.47)$$

This is compared with the isothermal susceptibility which is written as

$$\chi_{\mu\nu}^T = \int d\lambda \langle (M_\nu (-i\hbar\lambda) - \langle M_\nu \rangle)(M_\mu - \langle M_\mu \rangle) \rangle \quad (2.48)^*$$

The static susceptibility $\chi_{\mu\nu}(0)$ as given by (2.47) may, in fact, be called the susceptibility of the isolated system, since we pursued the natural motion of the system in deriving the equations. The question whether this should coincide with the isothermal susceptibility, or the adiabatic susceptibility of the magnetic body is a matter of which physical situation is under consideration. In order that $\chi_{\mu\nu}(0)$ gives $\chi_{\mu\nu}^T$, we have to take a large heat reservoir into our system. If we do this, we should expect that

$$\langle M_\nu^0 M_\mu^0 \rangle = \langle M_\nu \rangle \langle M_\mu \rangle$$

and the difference between Eqs. (2.47) and (2.48) will disappear. On the other hand, if we take the magnetic body only, then $\chi_{\mu\nu}(0)$ should be the adiabatic susceptibility rather than the isothermal. For a para-

* Eq. (2.48) is derived as follows:

$$\begin{aligned} \overline{M} &= \text{Tr} \{ e^{-\beta(H - \vec{H} \cdot \vec{M})} \vec{M} \} / \text{Tr} e^{-\beta(H - \vec{H} \cdot \vec{M})} \\ &= \{ \text{Tr} e^{-\beta H} (1 + \int_0^\beta d\lambda e^{\lambda H} (\vec{H} \cdot \vec{M}) e^{-\lambda H}) \vec{M} \} / \text{Tr} e^{-\beta H} + \sigma(\vec{H}) \\ &= \text{Tr}_0 \vec{M} + \text{Tr}_0 \int_0^\beta d\lambda e^{\lambda H} (\vec{H} \cdot \vec{M}) e^{-\lambda H} (\vec{M} - \langle \vec{M} \rangle) + \sigma(\vec{H}) \end{aligned}$$

magnetic body, the difference of the two susceptibilities vanishes as $\vec{H} \rightarrow 0$. In this case we may write (2.47) and (2.48) simply as

$$\chi_{\mu_0}^{\circ} = \int_0^{\infty} \langle M_0 (-i\hbar\lambda) M_\mu \rangle d\lambda . \quad (2.49)$$

This equation is a generalization of the famous Langevin-Debye equation, $\chi = N\mu^2/3kT$ which is given primarily for independent magnetic dipoles. This was generalized to interacting dipoles by Kirkwood⁸ and is expressed by

$$\begin{aligned} \chi &= \frac{\langle \vec{M}^2 \rangle}{3kT} , \quad \vec{M} = \sum \mu_i \\ \chi &= \frac{N \langle M_0 (\mu_0 + \sum_i \mu_i) \rangle}{3kT} = \frac{N \langle \mu_0 H_0^* \rangle}{3kT} . \end{aligned} \quad (2.50)$$

Eq. (2.49) is a quantum-mechanical form of this Kirkwood equation, and Eq. (2.46) is its generalization to dynamic susceptibility. Eq. (2.50) shows that the static susceptibility is a sum of space correlation of dipoles. The general dynamic susceptibility is expressed in terms of space-time correlation of magnetic dipoles.

2. Let us now consider electric conduction. The perturbation of the external electric field is now

$$H'_{ext}(t) = - \sum_i e_i \vec{r}_i \cdot \vec{E}(t) . \quad (2.51)$$

The response of the current component j_μ at the time t after a pulsive application of field E_0 is given by

$$\begin{aligned} \phi_{\mu_0}(t) &= \frac{1}{i\hbar} \text{Tr} [P, \sum_i e_i x_{i_0}] \sum_j e_j \dot{x}_{j\mu}(t) \\ &= \int_0^{\infty} \left\langle \sum_i e_i x_{i_0} (-i\hbar\lambda) \sum_j e_j \dot{x}_{j\mu}(t) \right\rangle d\lambda \\ &= \int_0^{\infty} \langle j_0 (-i\hbar\lambda) j_\mu(t) \rangle d\lambda \end{aligned} \quad (2.52)$$

where

$$j_\mu = \sum_i e_i \dot{x}_{i\mu} \quad (2.53)$$

is the current density. Therefore, the complex conductivity tensor for a periodic field is

$$\sigma_{\mu_0}(\omega) = \int_0^\infty e^{-i\omega t} dt \int_0^{\beta} d\lambda \langle j_\nu(-i\hbar\lambda) j_\mu(t) \rangle \quad (2.54)$$

In particular the static conductivity is given by

$$\sigma_{\mu_0} = \int_0^\infty dt \int_0^{\beta} d\lambda \langle j_\nu(-i\hbar\lambda) j_\mu(t) \rangle \quad (2.55)$$

The above treatment may easily be extended to a non-local relation of the current and the electric field. If the electric field is a function of space and time, i. e., $\vec{E} = \vec{E}(\vec{r}, t)$, the current density j will be written as

$$j_\mu(\vec{r}, t) = \iint K_{\mu_0}(\vec{r} - \vec{r}', \tau) \vec{E}(\vec{r}', t - \tau) d\vec{r}' d\tau \quad (2.56)$$

which is in general a linear equation and an expression of causality. The Fourier transform of (2.56), i. e.,

$$j_\mu(\vec{r}, \omega) = \int \bar{K}_{\mu_0}(\vec{r} - \vec{r}', \omega) E_\nu(\vec{r}', \omega) d\vec{r}' \quad (2.57)$$

gives the relation of current and field in a harmonic case. The kernel $K_{\mu_0}(\vec{r} - \vec{r}', \omega)$ is now expressed by

$$\bar{K}_{\mu_0}(\vec{r} - \vec{r}', \omega) = \int_0^\infty e^{-i\omega t} dt \int_0^{\beta} \langle j_\nu(\vec{r}, \omega) j_\mu(\vec{r}', t + i\hbar\lambda) \rangle d\lambda \quad (2.58)$$

More generally one may express the current as a linear function of the vector potential.

2.6. Dissipation-Fluctuation Theorem

In 1928, Niquist⁹ proved a theorem which states that the power spectrum of thermal noise in a resistive circuit is proportional to the absolute temperature and the proportionality constant is determined by the resistance at each frequency. This theorem has been discussed and extended by many people. I would like to mention here the work by Callen and Welton,¹⁰ who gave a general expression to this theorem using a perturbational method. Thus, Callen-Welton's proof of the generalized Niquist theorem, which is now called the dissipation-fluctuation theorem,

is essentially the same as that developed in this lecture, although here the expressions are more direct.

The dissipation-fluctuation theorem will be best explained for the conduction problem. Consider the expression (2.54) for the conductivity. Our task is to relate $\epsilon_{\mu\nu}(\omega)$ to the Fourier components of the correlation function

$$\Psi_{\mu\nu}(t) = \langle \{ j_\nu(0) j_\mu(t) \} \rangle \quad . \quad (2.59)$$

Half of this task has already been done by Eq. (2.40). The only thing left is to find the relation between $\epsilon_{\mu\nu}(\omega)$ and $f_{\mu\nu}(\omega)$, (2.39), which is given by

$$\begin{aligned} \epsilon_{\mu\nu}(\omega) &= \int_0^\infty \phi_{\mu\nu}(t) e^{-i\omega t} dt \\ &= \int_0^\infty e^{-i\omega t} dt \int_{-\infty}^\infty d\omega' f_{\mu\nu}(\omega') e^{i\omega t} \\ &\doteq \pi f_{\mu\nu}(\omega) + i \int_{-\infty}^\infty \frac{f_{\mu\nu}(\omega') d\omega'}{\omega' - \omega} \end{aligned} \quad (2.60)$$

Since we have $\overline{f_{\mu\nu}(\omega)} = f_{\nu\mu}(\omega)$ by Eq. (2.28), 2, we divide the tensor into symmetric and antisymmetric parts, $\epsilon_{\mu\nu}^s(\omega)$ and $\epsilon_{\mu\nu}^a(\omega)$.

It is now remembered that $\text{Re } \epsilon_{\mu\nu}^s(\omega)$ and $\text{Im } \epsilon_{\mu\nu}^s(\omega)$ are dissipative parts while $\text{Im } \epsilon_{\mu\nu}^a(\omega)$ and $\text{Re } \epsilon_{\mu\nu}^a(\omega)$ are nondissipative parts, because the latter components are concerned with the electric field which is out of phase with the current. For the dissipative parts, Eq. (2.60) gives the simple relations

$$\text{Re } \epsilon_{\mu\nu}^s(\omega) = \pi f_{\mu\nu}^s(\omega) , \quad \text{Im } \epsilon_{\mu\nu}^s(\omega) = \frac{\pi}{i} f_{\mu\nu}^a(\omega) \quad (2.61)$$

which, by Eq. (2.40), gives

$$E_\beta(\omega) \text{Re } \epsilon_{\mu\nu}^s(\omega) = \pi g_{\mu\nu}^s(\omega) = \int_0^\infty \Psi_{\mu\nu}^s(t) \cos \omega t dt \quad (2.62)$$

$$E_\beta(\omega) \text{Im } \epsilon_{\mu\nu}^s(\omega) = \frac{\pi}{i} g_{\mu\nu}^a(\omega) = - \int_0^\infty \Psi_{\mu\nu}^a(t) \sin \omega t dt$$

where $\Psi_{\mu\nu}^s$ and $\Psi_{\mu\nu}^a$ are the correlation functions

$$\Psi_{\mu\nu}^{s,a}(t) = \frac{1}{2} \langle \{ j_\nu(0) j_\mu(t) \pm j_\mu(0) j_\nu(t) \} \rangle , \quad (2.63)$$

which are even and odd in time respectively. Eq. (2.62) represents the Niquist-Callen-Welton theorem relating the dissipation to the thermal fluctuations.

It should be noted that the non-dissipative parts of the tensor cannot be related to the correlation spectra in such a simple way. This is because these parts are related to the dissipative parts by the Kramers-Kronig relations:

$$\text{Im} \sigma_{\mu_0}^s(\omega) = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{\text{Re} \epsilon_{\mu_0}^s(\omega')}{\omega' - \omega} d\omega' \quad (2.64)$$

$$\text{Re} \sigma_{\mu_0}^a(\omega) = - \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{\text{Im} \epsilon_{\mu_0}^a(\omega')}{\omega' - \omega} d\omega'$$

We can give complicated expression to express these non-dissipative parts by the correlation functions or their Fourier components, but this will be omitted here, except for noting the formula:

$$\sigma_{\mu_0}^a(0) = 2 \int_0^{\infty} \Psi_{\mu_0}^a(t) \int_0^t \Gamma(\tau) d\tau dt \quad (2.65)$$

On the other hand, Eq. (2.62) gives

$$\sigma_{\mu_0}^s(0) = \beta \int_0^{\infty} \Psi_{\mu_0}^s(t) dt \quad (2.66)$$

which is useful as a rigorous expression of static conductivity.

In the classical limit, $\hbar \rightarrow 0$, $E_p(\omega)$ in Eq. (2.62) simply goes to kT so that we have

$$\begin{aligned} \text{Re} \sigma_{\mu_0}(\omega) &= \int_0^{\infty} \Psi_{\mu_0}(t) \cos \omega t dt \\ \text{Im} \sigma_{\mu_0}(\omega) &= - \int_0^{\infty} \Psi_{\mu_0}(t) \sin \omega t dt \end{aligned} \quad (\text{classical}) \quad (2.67)$$

which includes dissipative and non-dissipative parts.

Similar theorems hold for any kind of admittance. For example, consider the magnetic susceptibility tensor,

$$\chi_{\mu_0} = \chi'_{\mu_0} - i \chi''_{\mu_0} \quad (2.68)$$

for which $\chi''_{s,\mu_0}(\omega)$ and $\chi'_{a,\mu_0}(\omega)$ are the dissipative parts. In particular, the energy absorption for a linearly polarized radiation is determined by

$$\begin{aligned}\chi''_{xx} &= \frac{\omega}{E_\beta(\omega)} \int_0^\infty \langle \{M_x(0)M_x(t)\} \rangle \cos\omega t dt \\ &= \frac{\omega}{2E_\beta(\omega)} \int_{-\infty}^\infty \langle \{M_x(0)M_x(t)\} \rangle \cos\omega t dt\end{aligned}\quad (2.69)$$

which may be approximated by

$$\chi''_{xx} = \frac{\omega}{2kT} \int_{-\infty}^\infty \langle \{M_x(0)M_x(t)\} \rangle \cos\omega t dt \quad (2.70)$$

if the important range of frequency lies in the region where

$$\hbar T \gg \hbar \omega \quad (2.71)$$

This is usually satisfied in magnetic resonance experiments.

Problem 4. With the use of Eq. (2.69), calculate the absorption spectrum of magnetic spins which are independently precessing in a constant magnetic field.

Problem 5. Consider a harmonic oscillator with the Hamiltonian

$$H = \frac{1}{2} P^2 + \frac{1}{2}(1+\alpha(t))q^2$$

where $\alpha(t)$ changes from 0 to α as t grows. Discuss this problem by perturbational method (Eq. (2.6)), assuming the initial distribution function is the form, $f(p,q) = f_0(\frac{1}{2}(p^2+q^2))$; $\alpha \ll 1$.

2.7. Moments and Sum Rules

It is interesting to note that the formal expression of admittance, Eq. (2.21), gives proof of certain general laws which we call the sum rules as a generalization of the well-known sum rule of the oscillator strength. For the admittance function, $\sigma(\omega)$, defined by

$$\sigma(\omega) = \int_0^\infty e^{-i\omega t} \phi(t) dt \quad (2.72)$$

we have the following relations:

1. If $\phi(t)$ is even in t , one finds

$$\phi(t) = \frac{1}{\pi} \int_{-\infty}^{\infty} e^{-i\omega t} R_e \Sigma(\omega) d\omega$$

so that the formulas

$$\begin{aligned}\phi(0) &= \frac{2}{\pi} \int_0^{\infty} d\omega R_e \Sigma(\omega), \quad \dot{\phi}(0) = -\frac{2}{\pi} \int_0^{\infty} \omega^2 d\omega R_e \Sigma(\omega) \\ (2.73)\end{aligned}$$

$$\phi^{(2n)}(0) = (-1)^n \frac{2}{\pi} \int_0^{\infty} \omega^{2n} d\omega R_e \Sigma(\omega)$$

hold. Also by integrating Eq. (2.72) partially, one gets

$$Im \Sigma(\omega) = -\frac{\phi(0)}{\omega} + \frac{\ddot{\phi}(0)}{\omega^3} - \frac{\dddot{\phi}(0)}{\omega^5} + \dots \quad (2.74)$$

2. If ϕ is odd in t , one finds

$$\phi(t) = \frac{1}{\pi i} \int_{-\infty}^{\infty} e^{i\omega t} Im \Sigma(\omega) d\omega$$

so that the equations

$$\begin{aligned}\dot{\phi}(0) &= \frac{2}{\pi} \int_0^{\infty} \omega d\omega Im \Sigma(\omega), \quad \ddot{\phi}(0) = -\frac{2}{\pi} \int_0^{\infty} \omega^3 d\omega Im \Sigma(\omega) \\ (2.75)\end{aligned}$$

$$\phi^{(2n+1)}(0) = (-1)^n \frac{2}{\pi} \int_0^{\infty} \omega^{2n+1} d\omega Im \Sigma(\omega)$$

hold. Corresponding to (2.74), one gets

$$R_e \Sigma(\omega) = -\frac{\dot{\phi}(0)}{\omega^2} + \frac{\ddot{\phi}(0)}{\omega^4} + \dots \quad (2.76)$$

These mathematical relations allow us to make the following state-

ment, which is a most general expression of the sum rules:

The initial values of time-derivatives of the response function generally determine the moments defined with respect to frequency distribution of the dissipative parts of admittance and also the coefficients of the series expansion of the non-dissipative parts in the inverse power of the frequency. In other words, these moments and the expansion coefficients are primarily determined by the static behavior of the system in equilibrium. It should be noticed here that the expansions (2.74) and (2.76) are not usual power series but are asymptotic expansions. This remark is very important.

We shall illustrate this theorem by the example of the conductivity tensor for a system of charged particles in a magnetic field, for which the Hamiltonian is

$$H = \sum_j \sum_i \frac{1}{2m_i} \left\{ P_{ij} - \frac{e_i}{c} A_j(\vec{r}_i) \right\}^2 + \bar{V}(\vec{r}_1 \dots \vec{r}_n) \quad (2.77)$$

\vec{A} being the vector potential. The velocity is defined by

$$v_{ij} = \frac{\pi_{ij}}{m_i} = \frac{1}{m_i} \left(P_{ij} - \frac{e_i}{c} A_j(\vec{r}_i) \right). \quad (2.78)$$

Let us assume that the static magnetic field is in the z -direction. Then we have the commutation law,

$$[\pi_{jx}, \pi_{jy}] = -\frac{\hbar}{i} \frac{e_j H}{c} \equiv -\frac{\hbar}{i} m_j \omega_j^o, \quad \omega_j^o = \frac{e_j H}{m_j c} \quad (2.79)$$

and the equation of motion,

$$\begin{aligned} \dot{\pi}_{jx} &= \omega_j^o \pi_{jy} - \frac{\partial V}{\partial x_j} & \pi_{jx} &= m_j \dot{x}_j \\ \dot{\pi}_{jy} &= -\omega_j^o \pi_{jx} - \frac{\partial V}{\partial y_j} & \pi_{jy} &= m_j \dot{y}_j \\ \dot{P}_{jz} &= -\frac{\partial V}{\partial z_j} & P_{jz} &= m_j \dot{z}_j \end{aligned} \quad (2.80)$$

By Eq. (2.52) we find

$$\begin{aligned}\dot{\phi}_{\mu\nu}(0) &= \frac{1}{i\hbar} \left\langle \left[\sum_j e_j x_{j\nu}, \sum_k \dot{x}_{k\mu} \right] \right\rangle \\ &= \sum_j \frac{e_j^2}{m_j} \delta_{\mu\nu} = \sum_r \frac{n_r e_r^2}{m_r} \delta_{\mu\nu}\end{aligned}\quad (2.81)$$

where r denotes the species of the charge carriers, n_r being the density of the r -th carrier. This follows from the commutation rule

$$[x_{j\nu}, \dot{x}_{k\mu}] = \frac{i\hbar}{m_j} \delta_{jk} \delta_{\mu\nu}$$

Using the commutation rules and the equation of motion, one may easily write down the expressions for the initial values of first few derivatives for the response functions*

$$\dot{\phi}_{\mu\nu}(0) = \sum_r \frac{n_r e_r^2}{m_r} \begin{bmatrix} 0 & \bar{\omega}_r & 0 \\ -\bar{\omega}_r & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \quad (2.82)$$

where

$$\begin{aligned}\bar{\omega}_r &= \sum_r \frac{n_r e_r^2}{m_r} \omega_r / \sum_r \frac{n_r e_r^2}{m_r} \\ \ddot{\phi}_{\mu\nu}(0) &= - \sum_r \frac{n_r e_r^2}{m_r} \begin{bmatrix} \bar{\omega}_r^2 & 0 & 0 \\ 0 & \bar{\omega}_r^2 & 0 \\ 0 & 0 & 0 \end{bmatrix} - \sum_j \sum_k \frac{e_j e_k}{m_j m_k} \left\langle \frac{\partial^2 V}{\partial x_{j\mu} \partial x_{k\nu}} \right\rangle\end{aligned}\quad (2.83)$$

where

$$\begin{aligned}\dot{\phi}_{\mu\nu}(0) &= \frac{1}{i\hbar} \left\langle [j_\mu, j_\nu] \right\rangle, & \ddot{\phi}_{\mu\nu}(0) &= \frac{1}{i\hbar} \left\langle [j_\mu, j_\nu] \right\rangle \\ \ddot{\phi}_{\mu\nu}(0) &= -\frac{1}{i\hbar} \left\langle [j_\mu, j_\nu] \right\rangle, & \phi_{\mu\nu}^{(IV)}(0) &= -\frac{1}{i\hbar} \left\langle [j_\mu, j_\nu] \right\rangle\end{aligned}$$

$$\begin{aligned}
 \overline{\omega_0}^2 &= \sum_r \frac{n_r e_r^2}{m_r} \omega_r^0 {}^2 / \sum_r \frac{n_r e_r^2}{m_r} \\
 \ddot{\phi}_{\mu\nu}(\omega) &= \sum_r \frac{n_r e_r^2}{m_r} \begin{bmatrix} 0 & -\overline{\omega_0}^3 & 0 \\ \overline{\omega_0}^3 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \\
 &\quad - \sum_j \sum_l \frac{\omega_j \omega_l}{m_j m_l} \begin{bmatrix} 0 & \left\langle \omega_l^0 \frac{\partial^2 V}{\partial x_j \partial x_l} + \omega_j^0 \frac{\partial^2 V}{\partial x_l \partial x_l} \right\rangle & \omega_j^0 \left\langle \frac{\partial^2 V}{\partial y_j \partial z_l} \right\rangle \\ -\left\langle \omega_l^0 \frac{\partial^2 V}{\partial z_j \partial x_l} + \omega_j^0 \frac{\partial^2 V}{\partial y_l \partial y_l} \right\rangle & 0 & -\omega_j^0 \left\langle \frac{\partial^2 V}{\partial x_j \partial z_l} \right\rangle \\ -\omega_j^0 \left\langle \frac{\partial^2 V}{\partial z_j \partial y_l} \right\rangle & \omega_j^0 \left\langle \frac{\partial^2 V}{\partial z_l \partial x_j} \right\rangle & 0 \end{bmatrix} \quad (2.84)
 \end{aligned}$$

where

$$\overline{\omega_0}^3 = \sum_r \frac{n_r e_r^2}{m_r} \omega_r^0 {}^3 / \sum_r \frac{n_r e_r^2}{m_r}$$

The simplest sum rule is now, according to Eq. (2.73),

$$\frac{2}{\pi} \int_0^\infty \text{Re} S_{\mu\nu}^s(\omega) d\omega = \sum_r \frac{n_r e_r^2}{m_r} S_{\mu\nu} \quad (2.85)$$

This reduces to the well-known sum rule for the oscillator strength as given in text books when applied to the system where the particles are moving independently. It should be particularly emphasized here that the sum rule as obtained in this form is quite general. It holds whatever the interactions of the particles are. It holds also irrespective of statistics and the temperature. This wide generality of the sum rule has not been fully recognized. One has to keep in mind the generality of similar sum rules discussed here.

For the non-dissipative part, corresponding to (2.85) we have

$$S_{\mu\nu}^s(\omega) \sim - \sum_r \frac{n_r e_r^2}{m_r \omega} S_{\mu\nu} \quad (\omega \rightarrow \infty) \quad (2.86)$$

This is easy to understand. At a very high frequency of the external field, only the inertia of the particles determines the response.

For the antisymmetric part we find the rules,

$$\frac{2}{\pi} \int_0^\infty \omega d\omega \text{Im} \epsilon_{xy}^a(\omega) = \sum n_r e_r^2 \frac{\omega_0}{m_r} \equiv \sum n_r e_r^2 H \quad (2.87)$$

and

$$\text{Re} \epsilon_{xy}^a(\omega) \sim - \sum \frac{n_r e_r^2}{m_r} \frac{\omega_0}{\omega^2} \quad (2.88)$$

The last result is also easily understood.

Further interesting results are obtained from Eqs. (2.83) and (2.84). In particular, we note the high frequency behavior of the non-dissipative part of the admittance, that determines the refractive index. Or, we may write the dielectric constant as

$$\epsilon \equiv \epsilon' - i\epsilon'' = 1 + \frac{4\pi \epsilon}{i\omega} \quad (2.89)$$

or as

$$\epsilon' = 1 + \frac{4\pi}{\omega} \text{Im} \epsilon \quad \epsilon'' = \frac{4\pi}{\omega} \text{Re} \epsilon$$

Thus, the high frequency behavior of $\text{Re} \epsilon$, and $\text{Im} \epsilon_a$ can be calculated in principle by knowing the statistical distribution of charges at equilibrium.

If the potential energy V is assumed to be

$$V = \sum v_{jl} (\vec{r}_j - \vec{r}_l) \quad (2.90)$$

then we have

$$\sum_j \sum_l \frac{e_j e_l}{m_j m_l} \left\langle \frac{\partial^2 V}{\partial x_{j\mu} \partial x_{l\nu}} \right\rangle = \sum_{j,l \text{ pairs}} \left(\frac{e_j}{m_j} - \frac{e_l}{m_l} \right)^2 \left\langle \frac{\partial^2 v_{jl}}{\partial x_{j\mu} \partial x_{l\nu}} \right\rangle$$

and

$$\sum_j \sum_l \frac{e_j e_l}{m_j m_l} w_j^0 \left\langle \frac{\partial^2 V}{\partial x_{j\mu} \partial x_{l\nu}} \right\rangle = \frac{H}{C} \sum_{j,l \text{ pairs}} \left(\frac{e_j}{m_j} - \frac{e_l}{m_l} \right)^2 \left(\frac{e_j}{m_j} - \frac{e_l}{m_l} \right) \left\langle \frac{\partial^2 v_{jl}}{\partial x_{j\mu} \partial x_{l\nu}} \right\rangle \quad (2.91)$$

These determine the terms which follow those given by Eqs. (2.86) and (2.88).

For simplicity, let us consider a plasma in which the free electrons are responsible for high frequency admittance. In this case, we obtain directly:

$$\mathcal{E}'_{xx} = \mathcal{E}'_{yy} \quad (2.92)$$

$$= 1 - \frac{4\pi n e^2}{m\omega^2} \left(1 + \frac{\omega_0^2}{\omega^2} + \frac{1}{m\omega^2} \left\langle \frac{\partial^2 \psi}{\partial x^2} \right\rangle + \dots \right)$$

$$\text{Re} \mathcal{G}_{xy} = \frac{n e^2 \omega_0}{m\omega^2} \left(1 + \frac{\omega_0^2}{\omega^2} + \frac{1}{m\omega^2} \left\langle \frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} \right\rangle + \dots \right) \quad (2.93)$$

$$(\omega_0 = \frac{eH}{mc}, \epsilon > 0)$$

where $\psi = \sum_i v_{i,\perp}$ is the potential of an electron in the force fields due to ions and neutral atoms, since the coulomb interaction between the free electrons automatically drops out from Eqs. (2.90), (2.91). Eq. (2.92) gives the correction to the critical frequency (plasma frequency) for the free electron value, i. e.,

$$\omega_\ell^2 = \omega_p^2 + \omega_0^2 + \frac{1}{3m} \langle \Delta \psi \rangle + \dots \quad (2.94)$$

$$(\omega_p^2 = 4\pi n e^2/m)$$

Similar considerations apply to other phenomena. For a magnetic body, we have

$$-\frac{2}{\pi} \int_0^\infty \text{Im} \chi_{\mu\nu}^s(\omega) \frac{d\omega}{\omega} = \chi_{\mu\nu}^s(\omega) \quad (2.95)$$

$$\frac{2}{\pi} \int_0^\infty \text{Im} \chi_{\mu\nu}^s(\omega) \cdot \omega d\omega = -\lim_{\omega \rightarrow \infty} \omega^2 \text{Re} \chi_{\mu\nu}^s(\omega)$$

$$= \frac{1}{i\hbar} \langle [M_\nu, \dot{M}_\mu] \rangle = \int_0^\infty \langle \dot{M}_\nu (i\hbar\lambda) \dot{M}_\mu \rangle d\lambda \quad (2.96)$$

$$\frac{2}{\pi} \int_0^\infty \text{Re} \chi_{\mu\nu}^a(\omega) d\omega = - \lim_{\omega \rightarrow \infty} \omega \text{Im} \chi_{\mu\nu}^a(\omega) = \frac{i}{\hbar} \langle [M_\mu, M_\nu] \rangle \quad (2.97)$$

and so forth. Some of these results are well known, but Eq. (2.97) is of particular interest. It gives

$$\frac{2}{\pi} \int_0^\infty \text{Re} \chi_{xy}^a(\omega) d\omega = - \lim_{\omega \rightarrow \infty} \omega \text{Im} \chi_{xy}^a(\omega) = - \sum_r \gamma_r \overline{M}_{rz} \quad (2.98)$$

where γ_r is the gyromagnetic ratio and \overline{M}_{rz} the average magnetization of r -th kind component of the system. This sum rule holds irrespective of the interaction present in the system.

Problem 6. The sum rule for electrons in a particular band is given by

$$\frac{2}{\pi} \int_0^\infty \text{Re} \Sigma_{\mu\nu}^s(\omega) d\omega = - \lim_{\omega \rightarrow \infty} \omega \text{Im} \Sigma_{\mu\nu}^s(\omega) = e^2 T_F \rho \frac{\partial^2 E}{\partial p_\nu \partial p_\mu}$$

where $E(\vec{p})$ is the energy of an electron with a crystal momentum \vec{p} . This sum rule holds when the interband transitions are omitted. Prove the above statement.

2.8. The Einstein Relation

It is interesting to note that the expression of conductivity, Eq. (2.55) involves the well-known Einstein relation

$$\mu = eD/kT$$

where μ is the mobility and D the diffusion constant. In order to see this, let us consider the simplest case where classical particles are moving independently. In this case, the general expression gives

$$\Sigma_{\mu\nu}^s = \frac{n e^2}{kT} \int_0^\infty \langle v_\nu(0) v_\mu(t) \rangle dt$$

Now we have

$$\int_0^\infty \langle U_\nu(0) U_\mu(t) \rangle dt = \lim_{T \rightarrow \infty} \frac{1}{2T} \int_0^T \int_0^T \langle U_\nu(t') U_\mu(t) \rangle dt dt' \quad (2.99)$$

$$= \lim_{T \rightarrow \infty} \frac{1}{2T} \int_0^T \langle (\chi_\nu(T) - \chi_\nu(0)) (\chi_\mu(T) - \chi_\mu(0)) \rangle = D_{\mu\nu}$$

by definition of diffusion constant. Therefore, we find the Einstein relation

$$\sigma_{\mu\nu}^s = n e^2 D_{\mu\nu} / kT \quad (2.100)$$

The most general form of the Einstein relation is given by

$$\sigma_{\mu\nu}^s = e^2 D_{\mu\nu} / \left(\frac{\partial \phi}{\partial n} \right) = \bar{\Delta n^2} \cdot e^2 D_{\mu\nu} \quad (2.101)$$

where ϕ is the chemical potential and $\bar{\Delta n^2}$ is the average fluctuation in the number density. This equation is valid for any system even in the presence of interaction or in a statistically degenerate state. For a classical system of independent particle $\bar{\Delta n^2}$ amounts to n/kT ; so Eq. (2.101) goes back to (2.100).

This general form of the Einstein relation is derived from the consideration that the gradients of electrostatic potential and chemical potential are combined together to determine the current. This holds generally for the symmetric part of the conductivity. It has been, however, pointed out by Kasuya and Nakajima (unpublished) that the anti-symmetric parts of the conductivity and the diffusion tensors may not be related by the Einstein relation. It is likely that the deviation from the Einstein relation becomes important at low temperatures and high magnetic field where quantum effects become predominant.

2.10. Electronic Conductivity Magnetic Field

As an example of application of the theory we shall here treat the problem of galvanomagnetic effect more in detail.¹¹ Let us consider the electrons in metals or in semiconductors, for which the band approximation is appropriate. The energy of an electron with the crystal momentum \vec{p} is denoted by $H_o(\vec{p})$. Neglecting for simplicity the possible effect of interband transitions we may write the effective Hamiltonian as¹²

$$H(\vec{p}, \vec{r}) = H_o(\vec{p}) + \vec{U}(\vec{r}) \quad (2.102)$$

where the quasi-momentum $\vec{\Pi}$ is defined by

$$\vec{\Pi} = \vec{P} + \frac{e}{c} \vec{A}(\vec{r}) , \quad (2.103)$$

\vec{A} being the vector potential of the magnetic field, and \vec{U} is the perturbation potential which causes the scattering of electrons. The interactions between electrons and ions of a perfect lattice and that between the electrons are assumed to have been taken into account by the band approximation.

The coordinate \vec{r} is not continuous but is primarily discrete to specify the expansion coefficients in the Wannier functions. However, we may treat it as continuous in good approximation. If the magnetic field \vec{H} lies in the z-direction, we have, by definition

$$[\Pi_x, \Pi_y] = \frac{\hbar e H}{ic} , \quad [\Pi_x, x] = [\Pi_y, y] = \frac{\hbar}{i} \quad (2.104)$$

$$\Pi_z \equiv P_z$$

and other usual commutators. The equation of motion is easily obtained from the assumed Hamiltonian (2.102), namely,

$$\begin{aligned} \dot{\Pi}_x &= -\frac{eH}{c} \frac{\partial H_0}{\partial \Pi_y} - \frac{\partial U}{\partial x} , & \dot{x} &= \frac{\partial H_0}{\partial \Pi_x} \\ \dot{\Pi}_y &= \frac{eH}{c} \frac{\partial H_0}{\partial \Pi_x} - \frac{\partial U}{\partial y} , & \dot{y} &= \frac{\partial H_0}{\partial \Pi_y} \\ \dot{P}_z &= -\frac{\partial U}{\partial z} , & \dot{z} &= \frac{\partial H_0}{\partial P_z} \end{aligned} \quad (2.105)$$

These equations are valid both classically and quantum-mechanically. We may now introduce the definition of the relative coordinate (ξ, η) and the center coordinate (X, Y) by

$$\begin{aligned} \xi &= \frac{c}{eH} \Pi_y , & \eta &= -\frac{c}{eH} \Pi_x \\ X &= x - \xi , & Y &= y - \eta \end{aligned} \quad (2.106)$$

for which we have

$$[\xi, \eta] = \frac{\hbar c}{ieH} \equiv \frac{e^2}{i} ; \quad [X, Y] = -\frac{\hbar c}{ieH} = -\frac{e^2}{i}$$

$$(l^2 \equiv \frac{\hbar c}{eH}). \quad (2.107)$$

Therefore, the set of variables (ξ, η) or (T_x, T_y) , (X, Y) , and (P_z, Z) is canonical. It is clear that the center coordinate (X, Y) remains constant if the perturbation is absent.* Then electrons will make spiral motion with constant P_z if the surface of constant energy

$$H_0(\vec{p}) = E$$

and the plane

$$P_z = \text{constant}$$

cut out a closed loop C in the momentum space. The projection C' of the spacial orbit C on to the x - y plane is then the same as C except the scale factor of c/eH and the rotation by 90 degrees.

Now the conductivity tensor is written as:

$$\Sigma_{\mu\nu} = e^2 \int_0^\infty dt \int_0^\theta d\lambda \langle v_\nu (-i\hbar\lambda) V_\mu(t) \rangle \quad (2.108)$$

where the gothic style means the operator in second quantization formalism, namely

$$v_\nu = \int \psi^+ v_\nu \psi dr$$

with the quantized wave functions ψ and ψ^+ . The velocity may be divided into two parts:

$$(V_\nu) = \begin{pmatrix} \dot{\xi} & + & \dot{X} \\ \dot{\eta} & + & \dot{Y} \end{pmatrix} \quad (2.109)$$

in the x - y plane. Therefore, the conductivity tensor may be expressed either in terms of the total velocity v , or in terms of the center displacement velocity (X, Y) and the relative velocity (ξ, η) . It can be shown that the first representation, which we call the v -representation, is

* By (2.105)

$$\dot{X} = \frac{c}{eH} \frac{\partial U}{\partial \eta}, \quad Y = -\frac{c}{eH} \frac{\partial U}{\partial \eta}$$

parallel to the classical theory or the usual treatment based on transport theory, and is convenient for weak field. Weak field here means a field H in which the electrons can rarely complete one cycle of screw motion before they are scattered ($\omega, \tau_r \ll 1$) $\omega \sim$ cyclotron frequency ($\tau_r \sim$ relaxation time). On the other hand, the second representation, which we briefly call the ξ -X-representation, is particularly convenient for strong field, where the electrons undergo a cyclotron motion, the scattering being relatively rare ($\omega, \tau_r \gg 1$). This is the region where the quantum effect is particularly important.

In the ξ -X-representation, we may expect generally that the conductivity tensor will consist of four parts including cross terms of relative and center velocities. It is, however, proved that as in the static conductivity, the cross terms vanish and a great simplification results. Thus the symmetric part is given by

$$\begin{aligned} \sigma_{\mu\nu}^S &= e^2 \int_0^\infty d\lambda \langle \dot{X}_\nu(-i\hbar\lambda) \dot{X}_\mu(t) \rangle \\ &= \frac{e^2 n c}{2kT} \int_0^\infty \langle \{\dot{X}_\nu(0) \dot{X}_\mu(t)\} \rangle dt, \quad (\mu, \nu) = (x, y) \end{aligned} \quad (2.110)$$

and the antisymmetric part by

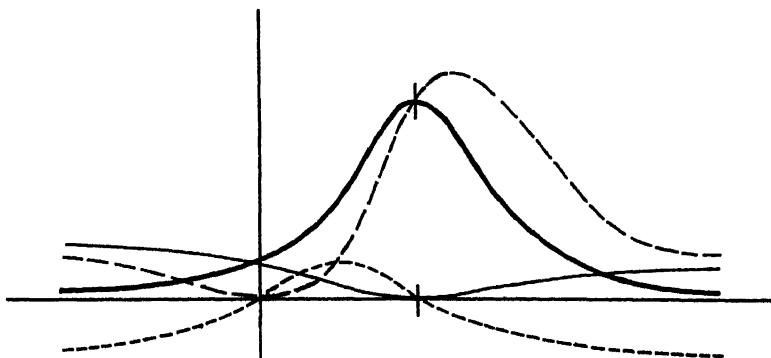
$$\sigma_{xy}^A = \frac{e n c}{H} + e^2 \int_0^\infty dt \int_0^\infty \langle \dot{Y}(-i\hbar\lambda) \dot{X}(t) \rangle d\lambda . \quad (2.111)$$

The real situation is most clearly understood when we consider the frequency dependent conductivity. Fig. 5 shows each component of $\sigma_{xy}(\omega)$ schematically. These curves correspond to the Fourier components of the correlation functions

$$\langle V_x(0) V_y(t) \rangle, \langle \dot{X}_x(0) \dot{X}_y(t) \rangle, \langle \dot{\xi}(0) \dot{\xi}(t) \rangle, \text{ and } \langle \dot{\xi}(0) \dot{X}_y(t) \rangle .$$

Only in the static case does $\langle \dot{X}(0) \dot{X}(t) \rangle$ give the whole conductivity. It is seen also from this figure that the v -representation primarily deals with the broadening of cyclotron resonance, the static conductivity being the tail of the broadened resonance at $\omega=0$.

Eq. (2.110) shows that the static conductivity is directly given by the Einstein relation in terms of the diffusion constant of the center coordinate. A jump of center takes place when the electron hits an impurity or a phonon. The diffusion constant has to be calculated by taking account of correlation of successive jumps. One sees at once that Eq. (2.110) allows a perturbational expansion, which actually corresponds to the expansion of



1. ——— $\int \langle v_i(0)v_i(t) \rangle e^{-i\omega t} dt$ 3. ——— $\int \langle \dot{\xi}(0)\dot{\xi}(t) \rangle e^{-i\omega t} dt$
 2. ——— $\int \langle \dot{x}(0)\dot{x}(t) \rangle e^{-i\omega t} dt$ 4. ——— $\int \langle \dot{\xi}(0)\dot{x}(t) \rangle e^{-i\omega t} dt$

Fig. 5 Fourier components of correlation functions of velocity components in magnetic field.

$$\frac{\gamma_r}{1 + \omega_0^2 \gamma_r^2} = \frac{1}{\omega_0^2 \gamma_r} - \frac{1}{\omega_0^4 \gamma_r^3} + \dots , \quad (2.112)$$

which appears in the classical expression for ζ_{xy} . For a high field ($\omega_0 \gamma_r \gg 1$) only the first term survives. This simplifies the consideration of the above mentioned correlation. In this limit (2.110) reduces essentially to

$$\zeta_{\mu\nu}^s = \frac{e^2 n_{eff}}{2kT} \left\langle \frac{\Delta X_\mu \Delta X_\nu}{\gamma} \right\rangle \quad (2.113)$$

where n_{eff} is the effective number of electrons per unit volume, $(\Delta X_\mu, \Delta X_\nu)$ is the displacement of the center during a scattering process and $1/\gamma$ is the probability of such scattering. Actual calculations may be done by direct use of (2.110) which may be written in matrix form as, e. g.

$$\zeta_{11} = \frac{e^2}{2kT} \left\langle \sum_n \sum_m f(\varepsilon_n)(1-f(\varepsilon_m)) |\langle n | \dot{x} | m \rangle|^2 \Delta_{mn} \right\rangle_{lattice} \quad (2.114)$$

where ξ_n is the electron energy and f is the Fermi distribution. The average over the lattice should be taken with respect to the phonon distribution or the random distribution of impurity scatterers (Δ_{nn} takes care of conservation of energy).

The first term of Eq. (2.111) comes from the relative motion, but it can be easily understood in terms of the equation of motion (2.105). It simply results from the drift in the magnetic field and gives the limiting value which is attained when the scattering becomes negligible. The second term of Eq. (2.111) can be interpreted in a similar way as that of the symmetric part.

The old theory of Titeica¹³ and the later theory of Davydow and Pomeranchuk¹⁴ are based on Eq. (2.110) although they established this by intuitive argument without noticing its full meaning. The writer and his collaborators have made calculations of the galvanomagnetic effect but the details have not yet been published.

2.11. Expression of Kinetic Coefficient for Thermal Disturbances

So far we have been talking about response of a system to an outer disturbance which is dynamical in nature, so that the disturbance could be explicitly expressed by a dynamical perturbation in the total Hamiltonian. There are, however, other kinds of external perturbations which are macroscopic in nature and so can not be uniquely expressed. For example, a difference in temperature or in chemical potential between two bodies in contact is a condition to be expressed in a statistical way but not in a dynamical way.

But we are rather convinced that the kinetic coefficients for this kind of thermal disturbances can also be expressed in terms of response functions or relaxation functions without relying upon the traditional method of setting up the transport equations. Because we now know that the conductivity, for instance, is given in such a form. If this is true, it is certainly a basis of the theory of irreversible processes. The role of such expressions is just like that of the expression of free energy in terms of a partition function. It may not be easy to calculate a kinetic coefficient from that type of expression. Furthermore, the physics lying at the bottom of such a formal expression is not necessarily easy to understand or even to give a rigorous justification.

Let us now consider a system which is macroscopically described by the variables $\{d_1, \dots, d_n\}$. As we have seen before, the kinetic coefficients L_{ij} are defined by Eq. (1.29) in a phenomenological way, and further they are related to the correlation of d_j and d_i in equilibrium by Eq. (1.34a). This is based on Onsager's assumption that the average regression of fluctuation follows the macroscopic law of irreversible process.

If we admit a priori this assumption we can easily obtain the expression for kinetic coefficients which may be used in quantum-mechanical systems.¹⁵ For this purpose we now define the initial state by a density matrix

$$\rho(0|\alpha') = \exp [\beta(\Omega - H) - \beta \sum A_j d_j]^{(2.115)}$$

which represents a statistical ensemble with the expectation values α'_j of d_j by properly chosen set of $\{A_j\}$. Thus,

$$\text{Tr } \rho(0|\alpha') d_j = \alpha'_j$$

The density matrix (2.115) is that which gives the maximum entropy for the given values of α'_j . Therefore we have

$$\beta \frac{\partial \Omega}{\partial A_j} = \bar{d}_j = \alpha'_j$$

$$S(\alpha'_1, \dots, \alpha'_n) = -k \beta \Omega + k \beta H + \sum k A_j \bar{d}_j$$

so that

$$\frac{\partial S}{\partial \alpha'_j} = k \beta A_j$$

Now we require by Onsager's assumption that

$$\frac{1}{\Delta t} \{ \text{Tr } \rho(\Delta t | \alpha') d_j - \alpha'_j \} = \sum L_{j\lambda} X_\lambda (\alpha') \quad (2.116)$$

corresponding to Eq. (1.31), where

$$\rho(\Delta t | \alpha') = e^{-i \Delta t H / \hbar} \rho(0, \alpha') e^{i \Delta t H / \hbar}.$$

The left-hand side is expanded in α'_j to their first order to give

$$\frac{1}{\hbar} \int_0^\theta \langle d_j(-i\hbar\lambda) \{ d_j(\Delta t) - d_j(0) \} \rangle d\lambda = -k G_{j\lambda} \Delta t. \quad (2.117)$$

This can be written as:

$$G_{j\lambda} = \frac{1}{k\beta} \int_0^{\Delta t} \left(1 - \frac{\tau}{\Delta t} \right) d\tau \int_0^\theta d\lambda \langle d_j(-i\hbar\lambda) d_j(\tau) \rangle, \quad (2.118)$$

where we used the condition

$$\int_0^{\beta} \langle \dot{d}_j (-i\hbar\lambda) d_j \rangle d\lambda = - \int_0^{\beta} \langle d_j (-i\hbar\lambda) \dot{d}_j \rangle d\lambda = 0 \quad (2.119)$$

which is satisfied in most practical cases.* Eq. (2.118) is derived from (2.117) by using the relation

$$\frac{d^2}{dt^2} \int_0^{\beta} \langle d_j (-i\hbar\lambda) d_j(t) \rangle d\lambda \quad (2.120)$$

$$= - \int_0^{\beta} \langle \dot{d}_j (-i\hbar\lambda) \dot{d}_j(t) \rangle d\lambda$$

and by integrating this twice with the use of (2.119).

Eq. (2.116) holds for a time interval so short in macroscopic scale to allow a linear decrease of the deviation from equilibrium and so long in microscopic scale that the macroscopic law applies. Therefore, (2.118) may be written as

$$G_{jj} = \frac{1}{\hbar \beta} \int_0^{\infty} dt \int_0^{\beta} d\lambda \langle \dot{d}_j (-i\hbar\lambda) \dot{d}_j(t) \rangle \quad (2.121)$$

provided that the correlation time of \dot{d}_j and \dot{d}_l is short enough compared to that of d_j and d_l which is governed by the macroscopic law and is measured by

$$\tau_{macro} = \langle d_j d_l \rangle / \hbar G_{jj} \quad (2.122)$$

In other words expressions of the type (2.121) are rigorous if such choice is possible to make τ_{macro} infinitely large. This is actually the case, as we shall see soon, for example, for those kinetic coefficients that enter in macroscopic conduction equations.

2.12. Derivation of Macroscopic Laws in Linear Dissipative Systems

In the foregoing argument, we trusted Onsager's assumption as our starting point. One may also take another way. Namely, we may pursue the actual change of macroscopic variables when the system is not in true equilibrium and find the law of the change. This is achieved

* Eq. (2.119) holds if $\langle [d_l, d_j] \rangle = 0$, that is if d_j and d_l commute on the average.

by a slight modification of the former treatment.¹⁶

Our system is now considered as macroscopically defined by a set of variables $\{d_1'(t), \dots, d_n'(t)\}$, $d_j'(t)$ being the macroscopically observed value of the corresponding dynamical quantity d_j at the time t . As before, we take $d_j' = 0$ ($j=1, \dots, n$) as the values in the state of true equilibrium. The state specified by $\{d_1', \dots, d_n'\}$ is not in true equilibrium but is in local equilibrium. Our first assumption here made is that the local equilibrium state is statistically represented by

$$\hat{\rho}_t \equiv \rho(d'(t)) = \exp\{\beta(\Omega - H) - \beta \sum A_j d_j\} \quad (2.123)$$

which is identical with (2.15), A_j being defined by the condition

$$\text{Tr } \rho(d'(t)) d_j = d_j'(t) \quad . \quad (2.124)$$

That is to say, $\{A_j\}$ and Ω in Eq. (2.123) changes in time so as to adjust the distribution to give the required time change of $\{d_j'(t)\}$. In this sense, $\hat{\rho}_t$, as defined by Eq. (2.123), is a function of time.

The time dependence of $d'(t)$ and hence that of $\hat{\rho}_t$ is not known yet. This is just what we want to find out. It should be kept in mind that the change of $\hat{\rho}_t$ in time is quite different from the dynamical development of the density matrix,

$$\rho(t+\tau | d'(t)) = e^{-i\tau H/\hbar} \hat{\rho}(d'(t)) e^{i\tau H/\hbar} \quad (2.125)$$

as the result of natural motion. In the following we shall write this as

$$\rho(t+\tau | d'(t)) \equiv \rho_t(t+\tau), \quad \rho_t(t+0) = \hat{\rho}_t \quad (2.126)$$

for the sake of brevity.

Eq. (2.125) gives now the change of average values of the d_j' s in the time period of τ , that is,

$$\overline{d_j(t+\tau)} = \text{Tr } \rho_t(t+\tau) d_j = \text{Tr } \hat{\rho}_t d_j(\tau) \quad . \quad (2.127)$$

The fundamental assumption we make here is that Eq. (2.127) can be used to determine the time dependence of $d_j'(t)$ for a time interval τ which is macroscopically short and microscopically long enough, i.e.,

$$\tau_{\text{micro}} \ll \tau_0 \sim \tau \ll \tau_{\text{macro}} \quad (2.128)$$

where τ_{macro} is the time over which the macroscopic variables change appreciably. The above assumption is expressed as:

$$\begin{aligned} \frac{d\dot{\alpha}_j(t)}{dt} &= \frac{1}{\tau} \left\{ \overline{\alpha_j(t+\tau)} - \dot{\alpha}_j(t) \right\} \\ &= \frac{1}{\tau} \text{Tr} \hat{\rho}_t \left\{ \dot{\alpha}_j(\tau) - \dot{\alpha}_j(0) \right\} . \end{aligned} \quad (2.129)$$

Therefore, with this assumption, we look at the system in the following way. We divide the time into short time intervals each being of the order τ_0 (2.128). Over each of these intervals, we let the density matrix follow its own course of natural motion. At the end of each interval, a readjustment is made to change the density matrix from the form (2.125) to $\rho(\alpha'(t+\tau)) = \hat{\rho}_{t+\tau}$. In doing so, the macroscopic parameters $\alpha'(t+\tau)$ are chosen to be equal to those values reached as the consequence of natural motion. This readjustment process sounds very artificial, but it is a way to represent the coarse-grained nature of our macroscopic observation.* There have been a great number of papers

* In fact, in order only to arrive at a result like (2.135), we may avoid such repeated readjustment procedures. The following logic may be employed. Namely, we consider the flow $\dot{\alpha}_j$ as a function of time t after the system starts from local equilibrium $\hat{\rho}$. The expectation of the flow is given by

$$J_j(t) = \text{Tr} \hat{\rho} \dot{\alpha}_j(t) ,$$

which reduces to

$$\begin{aligned} J_j(t) &= - \int d\lambda \text{Tr} \rho \sum A_m \alpha_m(-i\hbar\lambda) \dot{\alpha}_j(t) \\ &= - \sum_m A_m \int d\lambda \langle \alpha_m(-i\hbar\lambda) \dot{\alpha}_j(t) \rangle \\ &\quad + \sum_m A_m \int dt \int d\lambda \langle \dot{\alpha}_m(-i\hbar\lambda) \dot{\alpha}_j(t) \rangle d\lambda . \end{aligned}$$

Now the macroscopic current $J_j(t)$ will increase from zero to a certain value within a time period of the order of τ_{micro} , and it will keep practically constant for a time interval τ_0 , decaying thereafter with the relaxation time of the order of τ_{macro} .

With this consideration, the above equation shows that

$$L_{jm} = \frac{1}{\hbar} \left\{ \frac{1}{\tau_0} \int_0^t dt \int d\lambda \langle \dot{\alpha}_m(-i\hbar\lambda) \dot{\alpha}_j(t) \rangle d\lambda + \frac{i}{\hbar} \langle [\alpha_m, \alpha_j] \rangle \right\} .$$

This is identical with (2.135) except for the last term which is present unless the condition (2.119) is satisfied. It is noted here incidentally that this last term indicates the invalidity of Einstein's relation for the antisymmetric part of conductivity tensor mentioned in section 2.9.

discussing the problem of coarse-grained observation.¹⁷ None of them gets rid of the uneasy feeling of artificial construction, but it is reasonable to believe that the final answer does not depend critically on the type of argument. So we will not be much concerned with this, and will try to find any useful answers.

The treatment of Eq. (2.129) is naturally quite the same as that in the foregoing section. Namely, we expand $\rho(\lambda'(\tau))$ in the parameters $A_j(t)$ and get finally

$$\frac{d_j(t+\tau) - d_j'(t)}{\tau} = \sum_l A_l(t) \int_0^\tau (1 - \frac{t'}{\tau}) dt' \int_0^\theta d\lambda \langle d_l(-ih\lambda) d_j(t') \rangle \quad (2.130)$$

where we assumed for simplicity the condition (2.119). By the assumption of local equilibrium, we may define the entropy in local equilibrium, and then the force by

$$X_l(t) = \frac{\partial S}{\partial a'_l} = k\beta A_l(t) \quad (2.131)$$

which is conjugate to the flow

$$J_l = \dot{d}_l'(t) \quad (2.132)$$

Therefore, (2.130) may be written as

$$J_l = \frac{d d_l'}{dt} = \sum_m X_m L_{lm} \quad (2.133)$$

where L_{lm} is defined by the relation

$$L_{lm} = \frac{1}{k\beta} \int_0^\tau (1 - \frac{t'}{\tau}) dt' \int_0^\theta d\lambda \langle d_m(-ih\lambda) d_l(t') \rangle. \quad (2.134)$$

Now Eq. (2.133) is exactly the same as Eq. (1.27) of quasi-thermodynamics, with the kinetic coefficients defined by (2.134).

In order that this expression (2.134) have a value independent of τ , the correlation time of the integrand, which we call τ_c must be short, compared to τ_{macro} . * If this is the case, Eq. (2.134) may be simplified to

* That is to say, the integral (2.135) attains a plateau value for τ_c .
 $\tau_c \ll \tau_0 \ll \tau_{macro}$.

$$L_{jj} = \frac{1}{k_B} \int dt \int_0^{\infty} d\lambda \langle \dot{\phi}_j(-i\hbar\lambda) \dot{\phi}_j(t) \rangle \quad (2.135)$$

$(\tau_e \gg \tau_c \sim \tau_{\text{micro}})$

which is exactly the same as Eq. (2.121) except the upper limit of the time integral, which may, however, be put equal to infinity, if τ_{macro} can really be made infinitely large.

It is also possible to push a step further the parallelism of the present treatment and quasi-thermodynamics by introducing the entropy production. It is evident that $\hat{\rho}_t$ defined by (2.123) leads to a time-dependent entropy, and it changes exactly in the same way as we have seen in 1.2. But the problem is now how to define the entropy so that it increases as a direct result of the motion. According to Mori, this is possible through the definition,

$$S(t+\tau) = -k \text{Tr} \rho_t(t+\tau) \log \hat{\rho}_{t+\tau} \quad (2.136)$$

for a short time τ in the interval (2.127). Since the change of $\dot{\phi}'(t)$ is slow, (2.136) may well be approximated by

$$S(t+\tau) = -k \text{Tr} \rho_t(t+\tau) \log \hat{\rho}_t. \quad (2.137)$$

Eq. (2.136) or (2.137) may be written as

$$\begin{aligned} S(t+\tau) &= -\frac{1}{T} \text{Tr} \rho_t(t+\tau) \{ \Omega - H - \sum A_j(t+\tau) \phi_j \} \\ &= -\frac{1}{T} \text{Tr} \rho_t(t+\tau) \{ \Omega - H - \sum A_j(t) \phi_j \} \\ &= -\frac{1}{T} \text{Tr} \hat{\rho}_t \{ \Omega - H - \sum A_j(t) \phi_j(\tau) \} \end{aligned} \quad (2.138)$$

so that it defines the dynamical development of entropy. Following the assumption (2.129) we made previously for macroscopic quantities ϕ , we may now define the macroscopic increase of entropy by

$$\frac{dS}{dt} = \frac{1}{T} (S(t+\tau) - S(t)) .$$

Then we find at once from (2.138) and (2.129) that

$$\frac{dS}{dt} = \frac{1}{T} \sum A_j(\tau) \frac{dd'_j}{dt} = \sum X_j(t) \frac{dd'_j(t)}{dt} \quad (2.139)$$

$$= \sum_{\ell} X_{\ell} J_{\ell} .$$

This is the equation of entropy production (1.25).

Mori has shown that the definition of entropy by (2.137) satisfies the condition

$$S(t+\tau) > S(t) \quad (2.140)$$

which should hold for any reasonable definition of entropy. The proof of this goes in the following way. Since $\rho(t+\tau)$ is just a unitary transformation of ρ_t , we have

$$\text{Tr} \rho_t(t+\tau) \log \rho_t(t+\tau) = \text{Tr} \hat{\rho}_t \log \hat{\rho}_t .$$

Therefore we write

$$\begin{aligned} S(t+\tau) - S(t) &= -k [\text{Tr} \rho_t(t+\tau) \log \hat{\rho}_{t+\tau} - \text{Tr} \rho_t \log \hat{\rho}_t] \\ &\quad + k \text{Tr} \rho_t(t+\tau) \{ \log \hat{\rho}_{t+\tau} - \log \rho_t(t+\tau) \} \\ &= k \sum \langle m | \rho_t(t+\tau) | m \rangle \{ \langle m | \log \rho_t(t+\tau) | m \rangle - \langle m | \log \hat{\rho}_{t+\tau} | m \rangle \} \end{aligned}$$

where $\{ \langle m | \quad | m \rangle \}$ is the representation which diagonalizes $\rho_t(t+\tau)$. By the inequality*

$$\langle m | \log \rho_{t+\tau} | m \rangle \leq \log \langle m | \hat{\rho}_{t+\tau} | m \rangle$$

* For a hermitian operator A, the inequality

$$\langle m | \log A | m \rangle \leq \log \langle m | A | m \rangle$$

holds. The equality applies when and only when $\{ \langle m | \quad | m \rangle \}$ are the eigenvectors of A. This is seen from

$$\langle m | \log A | m \rangle = \sum_{\lambda} \log \alpha_{\lambda} / |\langle m | \lambda \rangle|^2$$

$$\log \langle m | A | m \rangle = \log \sum_{\lambda} \alpha_{\lambda} |\langle m | \lambda \rangle|^2, \quad A | \lambda \rangle = \alpha_{\lambda} | \lambda \rangle ,$$

and the concave property of logarithmic function.

We have now

$$\begin{aligned}
 S(t+\tau) - S(t) &\geq k \sum_m \langle m | \rho_t(t+\tau) | m \rangle \{ \log \langle m | \rho_t(t+\tau) | m \rangle - \log \langle m | \hat{\rho}_{t+\tau} | m \rangle \} \\
 &= k \sum_m \langle m | \rho_t(t+\tau) | m \rangle \{ \log \langle m | \rho_t(t+\tau) | m \rangle - \log \langle m | \hat{\rho}_{t+\tau} | m \rangle \} \\
 &\quad - \langle m | \rho_t(t+\tau) | m \rangle + \langle m | \hat{\rho}_{t+\tau} | m \rangle \\
 (\because \sum_m \langle m | \rho_t(t+\tau) | m \rangle = \sum_m \langle m | \hat{\rho}_{t+\tau} | m \rangle = 1).
 \end{aligned}$$

This is always positive unless $\rho_t(t+\tau) = \hat{\rho}_{t+\tau}$, because of the inequality

$$\chi(\log \alpha - \log \gamma) - \kappa + \gamma > 0, \quad \alpha \neq \gamma.$$

Thus we have proved that

$$S(t+\tau) - S(t) > 0.$$

The consideration made in this section is particularly useful, as shown by Mori, in order to find the appropriate quantities $\{\alpha_j\}$ to describe the phenomena we are concerned with. If we know a proper form of the local equilibrium density matrix (2.123) and write it as

$$\hat{\rho} = \rho(\lambda') = \exp \beta(\Omega - K) \quad (2.141)$$

we must have

$$R \equiv K - H = \sum_j A_j \alpha_j \quad (2.142)$$

where A'_j 's are usually such parameters introduced in the explicit expression of K to define the local equilibrium. Thus, the α_j 's in (2.142) are easily found from the assumed expression for K . Since the parameters A_j 's are essentially the forces, the flows conjugate to them are explicitly defined by

$$\dot{R} = \sum_j A_j \dot{\alpha}_j \quad (2.143)$$

and the expressions for the kinetic coefficients are just those given by (2.135).

2.13. Electron Transport Phenomena

The general consideration given in the two previous sections is now illustrated by the example of electron transport phenomena in solids. The phenomenological equations are:

$$\begin{aligned}\vec{j} &= \gamma^{(1)} (\vec{E} + \frac{1}{e} \nabla \xi) + \gamma^{(2)} \frac{1}{T} \nabla T \\ \vec{q} &= \gamma^{(3)} (\vec{E} + \frac{1}{e} \nabla \xi) + \gamma^{(4)} \frac{1}{T} \nabla T\end{aligned}\quad (2.144)$$

where \vec{j} is the electric current, \vec{q} the heat current, and ξ is S/T , S being the chemical potential. The coefficients $\gamma^{(1)} \dots \gamma^{(4)}$ are tensors of second rank for which we anticipate the following expressions:

$$\begin{aligned}S_{\mu\nu}^{(1)} &= \int_0^\infty dt \int_0^\beta d\lambda \langle j_\nu j_\mu(t + i\hbar\lambda) \rangle \\ S_{\mu\nu}^{(2)} &= \int_0^\infty dt \int_0^\beta d\lambda \langle q_\nu j_\mu(t + i\hbar\lambda) \rangle \\ S_{\mu\nu}^{(3)} &= \int_0^\infty dt \int_0^\beta d\lambda \langle j_\nu q_\mu(t + i\hbar\lambda) \rangle \\ S_{\mu\nu}^{(4)} &= \int_0^\infty dt \int_0^\beta d\lambda \langle q_\nu q_\mu(t + i\hbar\lambda) \rangle.\end{aligned}\quad (2.145)$$

These are just a straightforward extension of what we know about the electric conductivity.

1) First we shall follow the argument made in 2.12. The local equilibrium state is now defined by the distribution

$$\hat{\rho} = \exp [\beta \Omega - \int \beta(\vec{r}) \mathcal{E}(\vec{r}) d\vec{r} + \int g(\vec{r}) \eta(\vec{r}) d\vec{r}] \quad (2.146)$$

where

$$\mathcal{E}(\vec{r}) = \Psi^\dagger(\vec{r}) \mathcal{E}(\vec{r}) \Psi(\vec{r})$$

and

$$\eta(\vec{r}) = \Psi^\dagger(\vec{r}) \Psi(\vec{r})$$

are the energy density and the number density of electrons respectively. The local equilibrium is defined by the inhomogeneity of the distribution

of the temperature and the chemical potential, namely,

$$\begin{aligned}\beta(\vec{r}) &= 1/kT(\vec{r}) \\ \xi(\vec{r}) &= \xi(\vec{r})/kT(\vec{r}) .\end{aligned}\quad (2.147)$$

We denote the average of $\beta(\vec{r})$ and $\xi(\vec{r})$ over the space by β and ξ . Corresponding averages of $T(\vec{r})$ and $\xi(\vec{r})$ are denoted by T and ξ . Now R in Eq. (2.143) is given by

$$R = \int \left(\frac{\beta(\vec{r})}{\beta} - 1 \right) \dot{\mathcal{E}}(\vec{r}) d\vec{r} - \int \left(\frac{\xi(\vec{r})}{\xi} - 1 \right) \dot{n}(\vec{r}) d\vec{r}$$

which gives

$$\dot{R} = \int \left(\frac{\beta(\vec{r})}{\beta} - 1 \right) \dot{\mathcal{E}}(\vec{r}) d\vec{r} - \int \left(\frac{\xi(\vec{r})}{\xi} - 1 \right) \dot{n}(\vec{r}) d\vec{r}. \quad (2.148)$$

With the use of the continuity equation

$$\begin{aligned}\dot{n}(\vec{r}) &= \frac{1}{c} \nabla \cdot \vec{j}(\vec{r}) \\ \dot{\mathcal{E}}(\vec{r}) &= - \nabla \cdot \vec{q}(\vec{r}),\end{aligned}\quad (2.149)$$

Eq. (2.148) is transformed into

$$\dot{R} = \int \left\{ -\vec{q}(\vec{r}) \cdot \frac{1}{T} \nabla T + \vec{j} \cdot \frac{T}{e} \nabla \xi \right\} d\vec{r}. \quad (2.150)$$

This shows that the forces are the gradients of T and ξ , and the conjugate flows are \vec{q} and \vec{j} . Therefore, it is just a simple application of the theory of the foregoing section to write down Eq. (2.145) assuming that γ macro for the relaxation of ∇T and $\nabla \xi$ become infinity if the dimension of the system is made large enough. (The correlation times of \vec{j} and \vec{q} are finite, independently of the size of the system.)

2) The application of the method in 2.11 is not much different from the foregoing argument. The local equilibrium state is now considered as a state occurring as a fluctuation. The macroscopic variables are the energy density $\mathcal{E}(\vec{r})$ and the electron density $n(\vec{r})$, or more precisely, the Fourier components $\mathcal{E}_{\vec{k}}$ and $n_{\vec{k}}$. We may easily write down the entropy as a function of $\mathcal{E}_{\vec{k}}$ and $n_{\vec{k}}$ in the form

$$\begin{aligned} S &= S_o - \frac{1}{2T^2} \left(\frac{\partial T}{\partial \varepsilon} \right)_n V \sum_{\vec{k}} \dot{\varepsilon}_{\vec{k}} \varepsilon_{\vec{k}} \\ &\quad - \frac{1}{T^2} \left(\frac{\partial T}{\partial \eta} \right)_{\xi} V \sum_{\vec{k}} \dot{\eta}_{\vec{k}} \eta_{\vec{k}} \\ &\quad - \frac{1}{2} \left(\frac{\partial \xi}{\partial \eta} \right)_S V \sum_{\vec{k}} n_{\vec{k}} \eta_{\vec{k}} + \dots \end{aligned} \quad (2.151)$$

where V is the volume of the system under consideration.

In this argument, the flows are $\dot{\eta}_{\vec{k}}$ and $\dot{\varepsilon}_{\vec{k}}$ and the conjugate forces are $\frac{\partial \xi}{\partial \eta_{\vec{k}}}$ and $\frac{\partial \varepsilon}{\partial \varepsilon_{\vec{k}}}$. For these variables we have the linear relationship,

$$\begin{aligned} \dot{\eta}_{\vec{k}} &= -V \sum G_{\vec{k}\vec{k}'}^{(1)} \left\{ \left(\frac{\partial \xi}{\partial \eta} \right)_{\xi} \eta_{\vec{k}'} + \frac{1}{T^2} \left(\frac{\partial T}{\partial \eta} \right)_{\xi} \varepsilon_{\vec{k}'} \right\} \\ &\quad - V \sum G_{\vec{k}\vec{k}'}^{(2)} \left\{ \frac{1}{T^2} \left(\frac{\partial T}{\partial \eta} \right)_{\xi} \eta_{\vec{k}'} + \frac{1}{T^2} \left(\frac{\partial T}{\partial \varepsilon} \right)_{\eta} \varepsilon_{\vec{k}'} \right\} \\ \dot{\varepsilon}_{\vec{k}} &= -V \sum G_{\vec{k}\vec{k}'}^{(3)} \left\{ \left(\frac{\partial \xi}{\partial \eta} \right)_{\xi} \eta_{\vec{k}'} + \frac{1}{T^2} \left(\frac{\partial T}{\partial \eta} \right)_{\xi} \varepsilon_{\vec{k}'} \right\} \\ &\quad - V \sum G_{\vec{k}\vec{k}'}^{(4)} \left\{ \frac{1}{T^2} \left(\frac{\partial T}{\partial \eta} \right)_{\xi} \eta_{\vec{k}'} + \frac{1}{T^2} \left(\frac{\partial T}{\partial \varepsilon} \right)_{\eta} \varepsilon_{\vec{k}'} \right\} \end{aligned} \quad (2.152)$$

where

$$G_{\vec{k}\vec{k}'}^{(1)}, \dots, G_{\vec{k}\vec{k}'}^{(4)}$$

are the kinetic coefficients. Using Eq. (2.149) and

$$\nabla T = \frac{\partial T}{\partial \varepsilon} \nabla \varepsilon + \frac{\partial T}{\partial \eta} \nabla \eta, \quad \nabla \xi = \frac{\partial \xi}{\partial \varepsilon} \nabla \varepsilon + \frac{\partial \xi}{\partial \eta} \nabla \eta,$$

we find that (2.152) is identical with (2.144) if we put

$$\frac{1}{2} V G_{\vec{k}\vec{k}'}^{(r)} = \frac{T}{2} \vec{j}_{\vec{k}} \cdot \vec{\gamma}^{(r)} \vec{j}_{\vec{k}'} . \quad (2.153)$$

Now Eq. (2.117) gives

$$-J_{\vec{k}} G_{\vec{k}\vec{k}'}^{(r)} \Delta t = \frac{1}{\phi} \int_0^{\phi} \langle \eta_{\vec{k}'}(t-i\hbar\lambda) \{ \eta_{\vec{k}'}(t+\Delta t) - \eta_{\vec{k}'}(t) \} \rangle d\lambda$$

$$-\hbar G_{\vec{k}, \vec{k}}^{(2)} \Delta t = \frac{1}{\beta} \int_0^\beta \left\langle \sum_{-k} \{\eta_{-k}(t-i\hbar\lambda) \{ \eta_k(t+\Delta t) - \eta_k(t) \} \} \right\rangle d\lambda$$

(2. 154)

$$-\hbar G_{\vec{k}, \vec{k}}^{(3)} \Delta t = \frac{1}{\beta} \int_0^\beta \left\langle \eta_{-k}(t-i\hbar\lambda) \{ \varepsilon_k(t+\Delta t) - \varepsilon_k(t) \} \right\rangle d\lambda$$

$$-\hbar G_{\vec{k}, \vec{k}}^{(4)} \Delta t = \frac{1}{\beta} \int_0^\beta \left\langle \varepsilon_{-k}(t-i\hbar\lambda) \{ \varepsilon_k(t+\Delta t) - \varepsilon_k(t) \} \right\rangle d\lambda .$$

It is found easily that the condition (2.119) is satisfied in this case, because

$$\int_0^\beta \left\langle \eta_{-k}(t-i\hbar\lambda) \dot{\eta}_k(t) \right\rangle d\lambda = 0$$

$$\int_0^\beta \left\langle \varepsilon_{-k}(t-i\hbar\lambda) \dot{\varepsilon}_k(t) \right\rangle d\lambda = 0$$

$$\int_0^\beta \left\langle \dot{\eta}_{-k}(t-i\hbar\lambda) \varepsilon_k(t) \right\rangle d\lambda = \frac{1}{i\hbar} \left\langle [\eta_{-k}, \varepsilon_k] \right\rangle = -i\hbar \overline{j} = 0.$$

Furthermore, the decay time of the correlation of density fluctuations become infinitely long if the wavelength goes to infinity. Therefore, we have

$$\lim_{h \rightarrow 0} G^{(1)} = \lim_{h \rightarrow 0} \frac{1}{k\beta} \int_0^\infty dt \int_0^\beta d\lambda \langle \dot{\eta}_{-h}(-i\hbar\lambda) \dot{\eta}_h(t) \rangle$$

$$\lim_{h \rightarrow 0} G^{(2)} = \lim_{h \rightarrow 0} \frac{1}{k\beta} \int_0^\infty dt \int_0^\beta d\lambda \langle \dot{\epsilon}_{-h}(-i\hbar\lambda) \dot{\eta}_h(t) \rangle$$

(2.155)

$$\lim_{h \rightarrow 0} G^{(3)} = \lim_{h \rightarrow 0} \frac{1}{k\beta} \int_0^\infty dt \int_0^\beta d\lambda \langle \dot{\eta}_{-h}(-i\hbar\lambda) \dot{\epsilon}_h(t) \rangle$$

$$\lim_{h \rightarrow 0} G^{(4)} = \lim_{h \rightarrow 0} \frac{1}{k\beta} \int_0^\infty dt \int_0^\beta d\lambda \langle \dot{\epsilon}_{-h}(-i\hbar\lambda) \dot{\epsilon}_h(t) \rangle .$$

These equations give (2.145) with the aid of Eq. (2.149) and (2.153).

2.14. Energy Transfer between Two Systems

Let us consider the energy transfer process between two bodies which are in contact.¹⁶ If the coupling between the two is relatively weak and so each subsystem can be seen as nearly in equilibrium in itself, we are then treating a system which is nearly in a local equilibrium. This will change slowly in time through the flow of energy via the contact. We may then think of the effective heat conductivity of the contact. Problems of this sort are quite common in many relaxation processes.

We assume the total Hamiltonian of the composite system to consist of three parts.

$$H = H_1 + H_2 + H' \quad (2.156)$$

where H_1 and H_2 are Hamiltonians of the subsystems, 1 and 2, and H' is the interaction between them. Our basic assumption is that H' is small compared to H_1 and H_2 .

The local equilibrium is described by the temperatures T_1 and T_2 of the subsystems, for which we naturally assume that they deviate only little from the over-all temperature which should be realized in a true equilibrium. Therefore, the local equilibrium may be represented

by

$$\hat{\rho} = C \exp \left[- \left(\frac{H_1}{kT_1} + \frac{H_2}{kT_2} + \frac{H'}{kT_0} \right) \right] \quad (2.157)$$

$$\sim C \exp \left[- \left(\frac{H_1}{kT_1} + \frac{H_2}{kT_2} \right) \right].$$

The last term H'/kT_0 in the exponent is ambiguous, but it does not affect the answer in so far as H' is small enough. The function R (2.142) is now

$$R = - \frac{T_1 - T_0}{T_0} H_1 - \frac{T_2 - T_0}{T_0} H_2. \quad (2.158)$$

Therefore, the forces are the temperature deviations and the conjugate flows are the change of the energy of each system. Thus, the macroscopic change of U_1 , the energy of the subsystem of 1 is expressed as:

$$\frac{dU_1}{dt} = - L_{11} \frac{T_1 - T_0}{T_0} - L_{12} \frac{T_2 - T_0}{T_0} \quad (2.159)$$

from which we may easily write down the expressions for L_{11} and L_{12} . However, this can be simplified because the energy conservation law gives

$$\dot{H}_1 + \dot{H}_2 + \dot{H}' = 0 \quad \therefore \dot{H}_1 + \dot{H}_2 \sim 0$$

so that we have

$$L_{11} + L_{12} \sim 0.$$

Therefore (2.159) may be written as

$$-\frac{dU_1}{dt} = L^*(T_1 - T_2)/T_0 \quad (2.160)$$

with

$$L^* = \int_0^{T_0} dt \int_0^\theta \langle \dot{H}_1(-i\hbar\lambda) \dot{H}_1(t) \rangle d\lambda \quad (2.161)$$

where γ_0 must be long compared to the correlation time of the integrand and short on a macroscopic scale.

The crudest approximation of (2.161) is nothing but the result of simplest perturbational calculation.¹⁹ Taking the average by the local equilibrium distribution and taking the lowest order of perturbation, (2.161) is reduced to

$$\begin{aligned} L^* &= -\frac{1}{\hbar^2} \int_0^\infty dt \int d\lambda \text{Tr} \hat{\rho} e^{-\lambda(H_1+H_2)} [H_1, H'] e^{\lambda(H_1+H_2)} \\ &\quad e^{it(H_1+H_2)/\hbar} [H_1, H'] e^{-it(H_1+H_2)/\hbar} \end{aligned} \quad (2.162)$$

$$= \frac{1}{2\hbar^2 k T} \int_{-\infty}^{\infty} dt \text{Tr} \hat{\rho} [H_1, H'(0)] [H'(t), H_1]$$

where

$$H'(t) = e^{it(H_1+H_2)/\hbar} H e^{-it(H_1+H_2)/\hbar} \quad (2.163)$$

is the motion of the interaction looked upon from the frame moving with the natural motion of the subsystems 1 and 2.

Writing (2.162) in explicit matrix representation, one easily finds that this is the net rate of energy flow from 1 to 2 with the transition probability calculated by usual perturbation methods.

In particular, if the heat capacity of 2 is large compared to that of 1, (2.160) can be written as

$$\frac{dT_1}{dt} = -\frac{L^*}{C_1 T_0} (T_1 - T_0) \quad (2.164)$$

$(T_1 \sim T_0)$. Therefore, the relaxation time is defined by

$$\frac{1}{T_r} = \frac{L^*}{C_1 T_0} .$$

Further, if the temperature T_1 is so high that the heat capacity is given by

$$C_1 = \langle H_1^2 \rangle / \hbar T_r^2, \quad (2.165)$$

Eq. (2.162) gives

$$\frac{1}{T_F} = \frac{1}{2\hbar^2} \int_{-\infty}^{\infty} dt \left\langle [H_i, H'(0)] [H'(t), H_i] \right\rangle_0 / \left\langle |H_i|^2 \right\rangle_0 \quad (2.166)$$

where the subscript 0 means the average over the local equilibrium state. Although this equation is exactly the same as the simplest perturbation calculation, it is very useful for application.¹⁹

Problem 7. The system A is interacting with the other system B, which is in equilibrium represented by the density matrix ρ_B^0 . The transition probability of A from a state a' to a'' is given by

$$\overline{W}_{a', a''} = \frac{1}{\hbar^2} \int_{-\infty}^{\infty} dt e^{i\Delta E_A t/\hbar} \text{Tr}_B \rho_B^0 \langle a' | H' | a'' \rangle \langle a'' | H(t) | a' \rangle_B \quad (2.167)$$

where $\langle a' | H'(t) | a'' \rangle_B$ is regarded as changing in time due to the natural motion of B and $\Delta E_A = E_{a''} - E_{a'}$. Derive Eq. (2.164) using usual perturbation theory.

Problem 8. Apply (2.164) to the neutron scattering problem to express the scattering probability of the neutron from \vec{h} to \vec{h}' ($\vec{h}, \vec{h}':$ wave vectors) in terms of the space-time correlation function,

$$G(\vec{r}', \vec{r}; t) = \langle n(\vec{r}', 0) n(\vec{r}, t) \rangle$$

of the scattering particles.²⁰ For simplicity assume that the scattering system consists of one kind of particles. (This corresponds to the kinematical treatment of neutron diffraction phenomena.)

Problem 9. Derive the expression for viscosity coefficients similar to (2.145).

Problem 10. Suppose the electrons are nondegenerate, and are moving independently. Show that the general expression of conductivity gives

$$\sigma = \frac{e^2 n}{m} \tau \quad (2.168)$$

if the scattering is assumed to take place for each electron with mean free time τ_0 , and average $\langle \cos \theta \rangle$ of the cosine of the scattering angle. Thus

$$\tau = \tau_0 / (1 - \langle \cos \theta \rangle) .$$

Problem 11. Consider the degenerate electron system and derive Eq. (2.168). (Use the generalized equipartition law, $\langle (\sum_i \vec{p}_i^2)^2 \rangle = 3NmkT$ which holds irrespective of statistics and temperature.)

Problem 12. Discuss the relaxation process of nuclear magnetism in a

metal due to the Fermi-interaction of nuclear spins and the conduction electrons.²¹ (Assume the interaction to be of the form $H' = \sum_j \alpha \psi^*(\vec{R}_j) (\vec{I}_j \cdot \vec{\sigma}) \psi(\vec{R}_j)$ where \vec{I}_j and \vec{R}_j are the spin and position of j^{th} nucleus and $\vec{\sigma}$ is the spin operator for electron, ψ^* and ψ being quantized wave functions with two components.)

III. Further Remarks

There are many things left to be discussed further along the line of considerations made in this lecture. But time has passed so fast that I have to content myself by adding only a few remarks.

3.1. Magnetic Resonance Problem and the Concept of Motional Narrowing

1) The problems we usually meet here are calculations of the intensity distribution of resonance absorption and the relaxation time of liberation of the absorbed energy. As the theory is linear, we primarily neglect the saturation effect, but this can also be treated to a certain extent by introducing the spin-temperature which may not be equal to the bath temperature. The temperature difference can be determined by the condition of power balance.

The calculation of absorption intensity for linearly polarized radiation reduces, as shown by Eq. (2.70), to calculation of the correlation function.

$$\Phi(t) = \langle \{ M_x(0) M_x(t) \} \rangle \quad (3.1)$$

In an ideally simple case of independent spins, each having definite surrounding, calculation of (3.1) or more directly that of the resonance spectrum is simply a determination of the energy levels and the matrix elements of M_x . A more complicated situation arises if the surroundings are not definite but are changing in time, or if the spins are interacting with each other.

Explicit calculations for such complicated systems are usually not very easy, depending on the type of interaction present. Most straightforward calculations can be made along the line of arguments made in 2.7. This is the so-called moment method. The moments of lower order may be calculated from the explicit form of the interaction. There is, however, a complexity about this moment method.²² In magnetic resonance problems, the moments to be measured by experiments are defined with respect to the main lines which are determined by the external magnetic field and other dominant interactions. But the moments as defined by (2.73) are primarily defined for the whole region of frequency. The satellite lines may be weak but they are far apart from the main lines so that they usually contribute definite amounts to the total moments. Elimination of these satellite parts from the calculation makes the calculation rather complicated. It becomes very tedious to calculate the moments higher than say, the fourth.

2) Although a quantitatively exact calculation of (3.1) is very difficult for any real system, a qualitative consideration of (3.1) for some simplified models is very useful to help our understanding of the laws of nature.

The simplest model is that the total magnetic moment consists of independent components, each of which is moving by the equation of motion,

$$\dot{\vec{m}} = (\vec{\omega}_0 + \vec{\omega}') \times \vec{m} \quad (3.2)$$

where the torque $\vec{\omega}_0 \times \vec{m}$ comes from a constant external field and $\vec{\omega}' \times \vec{m}$ is produced by the surroundings of the magnetic moment in question. Thus, $\vec{\omega}'$ is the local field. Thus, we are led to a simple stochastic model of the magnetic resonance problem if we assume the local field $\vec{\omega}'$ is a random variable, changing from one spin to another and also changing in time because of the motion of the surroundings. Assuming further, for simplicity, that the local field $\vec{\omega}'$ is always parallel (this is not true in actual cases) to the constant field $\vec{\omega}_0$, the calculation of (3.1) is now reduced to the following problem.

Consider a stochastic variable $\chi(t)$ which follows the equation of motion

$$\dot{\chi}(t) = i(\omega_0 + \omega'(t)) \chi(t) \quad (3.3)$$

and hence changes in time as

$$\chi(t) = \chi(0) e^{i\omega_0 t + i \int_0^t \omega'(t') dt'} \quad (3.4)$$

The correlation function of $\chi(t)$ is defined by

$$\langle \chi(t) \chi(0) \rangle = \langle \chi(0)^2 \rangle e^{i\omega_0 t} \langle e^{i \int_0^t \omega'(t') dt'} \rangle \quad (3.5)$$

$$= \langle \chi(0)^2 \rangle e^{i\omega_0 t} \phi(t)$$

$$\phi(t) = \langle e^{i \int_0^t \omega'(t') dt'} \rangle \quad (3.6)$$

The problem is to find $\phi(t)$ when the stochastic law is known for the variable $\omega'(t)$ which is naturally assumed to be ergodic. When $\phi(t)$ is found, the intensity distribution $I(\omega)$ is calculated from its definition

$$I(\omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \phi(t) e^{-i\omega t} dt . \quad (3.7)$$

This gives the intensity distribution of the broadened resonance line, ω being measured as the deviation from the center. We call this problem the stochastic model of magnetic resonance.²³⁻²⁵

We may now assume that

$$\langle \omega'(t) \rangle = 0 \quad (3.8)$$

since we have only to shift the center ω_0 to $\omega_0 + \langle \omega' \rangle$ if $\langle \omega' \rangle$ does not vanish. We choose the correlation time of $\omega'(t)$ defined by

$$\tau_c = \int_0^{\infty} \langle \omega'(t) \omega'(t+\tau) \rangle d\tau / \langle \omega'^2 \rangle \quad (3.9)$$

as the measure of rapidity of the stochastic change of $\omega'(t)$. Two extreme cases are now easily to be seen.

a) τ_c is very large, that is to say, $\omega'(t)$ changes very slowly. This may be said to be a static case. The line shape, (3.7), represents directly the distribution of the local field ω' . Namely

$$I(\omega) = P_o(\omega) \quad (3.10)$$

where $P_o(\omega)$ is the distribution function of the random variable ω' .

b) τ_c is very short, namely $\omega'(t)$ changes very rapidly. Then the effect of the perturbation will just average out and the line shape approaches to a sharp line

$$I(\omega) \rightarrow \delta(\omega) . \quad (3.11)$$

Therefore the question is now what should be compared to τ_c to determine whether τ_c is short or long. The answer to this is given by the conditions

$$\begin{aligned} \text{a)} \quad \Delta &\equiv \langle \omega'^2 \rangle^{1/2} \gg \frac{1}{\tau_c} \\ \text{b)} \quad \Delta &\equiv \langle \omega'^2 \rangle^{1/2} \ll \frac{1}{\tau_c} \end{aligned} \quad (3.12)$$

which characterizes the two extreme cases mentioned in the above. The general trend of the change of the line shape (3.7) is shown in the Fig. 6, where the breadth of the line is drawn as a function of γ_e . The decrease of the width, or the sharpening of the resonance line, caused by the rapid change of perturbation is called the motional narrowing. This concept has been introduced by Bloembergen, Purcell, and Pound²⁶ in the analysis of their experiment of nuclear magnetic resonance in liquids. The

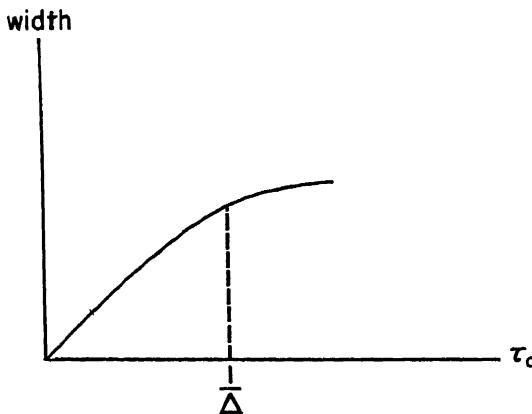


Fig. 6

idea of exchange narrowing phenomena in paramagnetic resonance is also basically the same.²⁷

In order to make a quantitative description of the motional narrowing as γ_e decreases from ∞ to 0, we have to know more detailed nature of the stochastic variables $\omega'(t)$. Specification of γ_e (3.9), is not enough. There are two typical models which allow exact mathematical treatment.

A) Gaussian process:²⁸ This means that the distribution law of the variables $\omega'(t_1), \dots, \omega'(t_n)$ for arbitrary n time points is always Gaussian. Physically, this situation is realized if the local field ω' consists of a number of small components, i. e.,

$$\omega' = \sum_{j=1}^N \Delta \omega_j' \quad N \gg 1 \quad (3.13)$$

as an extension of the well-known central limit theorem. Under the assumption of a Gaussian process, we can easily prove that the correlation

function $\phi(t)$, Eq. (3.6) is given by*

$$\begin{aligned}\phi(t) &= \exp \left[-\int_0^t (t-\tau) \langle \omega'(0) \omega'(\tau) \rangle d\tau \right] \\ &= \exp \left[-\Delta^2 \int_0^t (t-\tau) \Psi_{\omega'}(\tau) d\tau \right]\end{aligned}\quad (3.14)$$

where the correlation function $\Psi_{\omega'}$ of $\omega'(t)$ is defined by

$$\Psi_{\omega'}(\tau) = \langle \omega'(t) \omega'(t+\tau) \rangle / \langle \omega'^2 \rangle \quad (3.15)$$

for which we have, by (3.9),

* Let us define

$$g_N(\xi) = \left\langle \exp \left[i \sum_{k=1}^N \xi_k \omega'(t_k) \right] \right\rangle \equiv \left\langle \exp(i \vec{\xi} \vec{\omega}') \right\rangle$$

which is the characteristic function for the distribution function of $\omega'(t_1)$ and $\omega'(t_N)$, $\vec{\xi}$ and $\vec{\omega}'$ being the vectors (ξ_1, \dots, ξ_N) , and $(\omega'(t_1), \dots, \omega'(t_N))$. Since the distribution is gaussian by definition, we have

$$g_N(\xi) = \exp \left[-\frac{1}{2} \vec{\xi} A \vec{\xi} \right]$$

where A is the correlation tensor

$$A_{lm} = \langle \omega'(t_l) \omega'(t_m) \rangle / \langle \omega'^2 \rangle.$$

Putting $\xi_k t_k/N = S$ and letting $S \rightarrow 0$ we have

$$g_N \rightarrow \phi(t) = \exp \left\{ -\frac{1}{2} \int_0^t \int_0^t \langle \omega'(t_1) \omega'(t_2) \rangle dt_1 dt_2 / \langle \omega'^2 \rangle \right\}$$

which gives (3.14) by virtue of the stationarity condition

$$\langle \omega'(t_1) \omega'(t_2) \rangle = \langle \omega'(0) \omega'(t_2 - t_1) \rangle = \langle \omega'(t_1 - t_2) \omega'(0) \rangle$$

$$\Upsilon_c = \int_0^\infty \Psi_{\omega'}(\tau) d\tau . \quad (3.16)$$

Explicit calculations of $\phi(t)$ by (3.14) can be made if $\Psi_{\omega'}(\tau)$ is known.

Let us examine by this model the two extreme cases mentioned before. In the first place, in the limit of a static perturbation, we have apparently a Gaussian distribution for the intensity with the width Δ^2 . Thus, we may expect the important frequency range for $I(\omega)$ is Δ and therefore the important time scale is of the order of $1/\Delta$.

If $\Psi_{\omega'}(\tau)$ changes very little in the time interval $1/\Delta$ (i.e., $\Upsilon_c \gg 1/\Delta$), we may put $\Psi_{\omega'}(\tau) \sim \Psi_{\omega'}(0) = 1$ in the integral in Eq. (3.14) without making any serious error in the important range of t . Thus, we have

$$\phi(t) \sim \exp \left\{ -\frac{\Delta^2}{2} t^2 \right\} \quad (3.17)$$

as the static limit. The Fourier transform of this gives, of course, a Gaussian line.

On the contrary, if $\Psi_{\omega'}(\tau)$ decays very fast during the time interval of our concern, Eq. (3.14) gives

$$\phi(t) \sim \exp [-t \Upsilon_c \Delta^2] \quad (\Upsilon_c \Delta \ll 1) \quad (3.18)$$

as the narrowing limit. This gives a Lorentzian line

$$I(\omega) \sim \frac{1}{\pi} \frac{1}{\omega^2 + (\Upsilon_c \Delta^2)^2} \quad (3.19)$$

with the halfwidth

$$\Upsilon_c \Delta^2 = \Delta \times (\Upsilon_c \Delta) \quad (3.20)$$

$\Upsilon_c \Delta$ being the narrowing ratio.

B) Markoffian process: In this model we assume that the local field ω' is changing in time via a Markoffian process. In order to make the statement simpler let us assume that the values of ω' are discrete which will be denoted by ω'_k ($k=1, \dots, r$). As a stationary Markoffian process, the change of probability $P_j(t)$ to find ω' in the state ω'_j is governed by the equation

$$\frac{dP_j}{dt} = -C_j P_j + \sum_k P_k C_k P_{kj} = -\sum_k D_{kj} P_k \quad (3.21)$$

where C_j is the reciprocal life time of the j -th state and p_{kj} is the transition probability. It is now shown that $\phi(t)$, Eq. (3.6), is then determined by the equation

$$\begin{aligned} \phi(t) &= \sum_j u_j(t) \\ \left(\frac{d}{dt} - i\omega_j \right) u_j(t) + \sum_k D_{kj} u_k(t) &= 0 \quad (3.22) \\ u_j(0) &= P_j^0 \end{aligned}$$

where P_j^0 is the equilibrium distribution ($\sum_k D_{kj} P_k^0 = 0$). The general discussion of this model is more complicated than that of a Gaussian process, so that we shall not discuss it further. But we can show a similar behavior of $\phi(t)$ and $I(\omega)$ in the above-mentioned extreme cases.²⁴

It should be noticed here that, if we confine ourselves to the limit of motional narrowing, we may show the general trend without referring to particular assumptions such as Gaussian or Markoffian character of the perturbation. It seems to the writer very important to recognize this, since our argument shares rather general features with other problems of irreversible processes and also with many of quantum-mechanical treatments of scattering and many-body problems even though they are not usually viewed from such a point of view.

3) Returning to Eq. (3.2), or rather to

$$\dot{\chi}(t) = i\omega'(t) \chi(t) \quad , \quad (3.23)$$

we shall show that the average regression of χ follows a simple exponential decay in the motional narrowing limit. We shall do it in two ways. From Eq. (3.23) we have

$$\begin{aligned} &\phi(t+\tau) - \phi(t) \\ &= \langle \chi(0) \chi(t+\tau) \rangle - \langle \chi(0) \chi(t) \rangle \\ &= \langle \chi(0) \chi(t) \left\{ e^{i \int_t^{t+\tau} \omega'(t') dt'} - 1 \right\} \rangle \quad (3.24) \\ &= \langle \chi(0) \chi(t) \left\{ i \int_t^{t+\tau} \omega'(t') dt' - \frac{1}{2} \int_t^{t+\tau} \int_t^{t+\tau} \omega'(t') \omega'(t'') dt' dt'' + \dots \right\} \rangle \end{aligned}$$

Now the assumption is that the correlation time τ_c of $\omega'(t)$ is very short compared to the time constant τ_r which characterizes the decay of $\phi(t)$.

With this assumption τ in (3.24) is chosen in the range

$$\tau_c \ll \tau \quad (3.25a)$$

$$\tau \ll \tau_r . \quad (3.25b)$$

By (3.25b) the left hand side of Eq. (3.24) may be replaced by the real derivative. By (3.25a) the average on the right-hand side can be split into

$$\begin{aligned} & \langle \chi(0) \chi(t) \rangle \left\langle i \int_t^{t+\tau} \omega'(t') dt' - \frac{1}{2} \int_t^{t+\tau} \int_t^{t+\tau} \omega'(t') \omega'(t'') dt' dt'' + \dots \right\rangle \\ &= -\phi(t) \int_0^{\tau} (\tau - t') \langle \omega'(t'') \omega'(t'' + t') \rangle dt' + \dots . \end{aligned} \quad (3.26)$$

Therefore, Eq. (3.24) can be written as

$$\frac{d\phi}{dt} = -\frac{\phi}{\tau} \int_0^{\tau} (\tau - t') \langle \omega'(t'') \omega'(t'' + t') \rangle dt' = -\phi/\tau_r \quad (3.27)$$

where

$$\begin{aligned} \frac{1}{\tau_r} &= \frac{1}{\tau} \int_0^{\tau} (\tau - t') \langle \omega'(t'') \omega'(t'' + t') \rangle dt \\ &\approx \int_0^{\infty} \langle \omega'(t'') \omega'(t'' + t') \rangle dt' = \tau_c \Delta^2 \end{aligned} \quad (3.28)$$

gives the relaxation time of ϕ . The condition (3.25) can be fulfilled if

$$\tau_c \ll \tau_r$$

or

$$\tau_c \Delta \ll 1 . \quad (3.29)$$

Relation (3.29) is the condition mentioned in (3.13). If (3.29) holds, then $\phi(t)$ decreases with t following Eq. (3.27) for the time region

$$t \gg \tau_c . \quad (3.30)$$

To be a little more exact, one has to examine more carefully the higher order terms in Eq. (3.26). Let us consider for example the fourth order term. The average of this term will consist of terms of the order

$$(1) \quad \tau^2 (\Delta^2 \tau_c^2) \quad \text{and} \quad (2) \quad \tau \Delta^4 \tau_c^3 .$$

The first term is of high order, since

$$\tau^2 (\Delta^2 \tau_c^2)^2 = \tau^2 / \tau_r^2 \ll \tau / \tau_r .$$

The second term is

$$\tau \Delta^4 \tau_c^3 = \tau (\Delta^2 \tau_c^2)^2 \times \tau_c = \tau \tau_c / \tau_r^2 \ll \tau / \tau_r .$$

In the similar way, we can show that (3.27) correctly describes the correlation function if (3.29) is satisfied. This argument of motional narrowing does not depend on any particular assumption for the stochastic nature of $\omega'(t)$. It should be noticed here that the logic involved is essentially the same as that which was used in (2.11) and (2.12), although there we did not examine things in any great detail. Another way of obtaining

$$\phi(t) = e^{-t/\tau_r} \quad (3.31)$$

from

$$\phi(t) = \left\langle e^{i \int_0^t \omega'(t') dt'} \right\rangle \quad (3.32)$$

is to use the direct expansion.

$$\begin{aligned} \phi(t) &= \left\langle 1 + i \int_0^t \omega'(t_1) dt_1 + i^2 \iint_0^t \omega'(t_1) \omega'(t_2) dt_1 dt_2 \right. \\ &\quad \left. + \cdots + i^n \int_0^t \int_0^{t_n} \cdots \int_0^{t_2} \omega'(t_1) \omega'(t_2) \cdots \omega'(t_n) dt_1 \cdots dt_n \right\rangle \end{aligned} \quad (3.33)$$

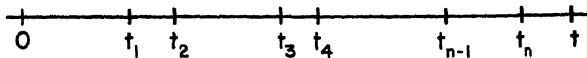


Fig. 7

Now, a general term $n = 2m$ will give the main term

$$(-1)^m \int_0^t \cdots \int_0^{t_3} dt_2 \int_0^{t_2} dt_1 \langle \omega'(t_1) \omega'(t_2) \rangle \langle \omega'(t_3) \omega'(t_4) \rangle \cdots \langle \omega'(t_{2m-1}) \omega'(t_{2m}) \rangle \quad (3.34)$$

In this integrand t_{2j-1} and t_{2j} must be nearby with the distance of the order τ_c in order to secure a finite value of the integrand. Thus, (3.34) is nearly equal to

$$\begin{aligned} & (-1)^m \int_0^t dt_{2m-1} \int_0^t dt_{2m-3} \cdots \int_0^{t_s} dt_1 \int_0^{\infty} \langle \omega'(t_1) \omega'(t_1 + \tau_c) \rangle d\tau_c \cdots \int_0^{\infty} \langle \omega'(t_{2m-1}) \omega'(t_{2m-1} + \tau_c) \rangle d\tau_c \\ & = (-1)^m \frac{t^m}{m!} (\Delta^2 \tau_c)^m. \end{aligned}$$

Picking up only these contributions (3.33) is approximated by

$$\phi(t) = e^{-t\Delta^2 \tau_c} \equiv e^{-t/\tau_c}.$$

Other terms can be shown to be safely neglected if

$$t \sim \tau_c \gg \tau_c$$

which is essentially the same as before. The resemblance of (3.33) to the expansion of quantum-mechanical transformation function,

$$\begin{aligned} & e^{iHt/\hbar} \equiv e^{i(H_0+H')t/\hbar} \\ & = e^{iH_0 t/\hbar} \left\{ 1 + \frac{i}{\hbar} \int_0^t H'(t_1) dt_1 + \left(\frac{i}{\hbar}\right)^2 \iint_0^t H'(t_1) H'(t_2) dt_1 dt_2 + \cdots \right\} \quad (3.35) \end{aligned}$$

should particularly be noted here. Van Hove's theory²⁹ of the asymptotic form of (3.35) follows a very similar development to that used here, although there the mathematics takes a more complicated form.

We might add another remark. The derivation of the asymptotic form (3.31) from (3.23) does not mean that the simple exponential decay is always expected for any correlation function. Generally the decay will be a superposition of exponential functions with a number of relaxation constants. A model which leads to such a behavior is given by

$$\dot{\chi}_j(t) = i \sum \omega'_{jk}(t) \chi_k(t) \quad (3.36)$$

where $\omega'_{jk}(t)$ are also considered as stochastic variables. The integration of (3.36) may be expressed as

$$\vec{\chi}(t) = \left[\exp i \int_0^t \Omega(t') dt' \right]_+ \vec{\chi}(0) \quad (3.37)$$

where $[\exp]_+$ is the ordered exponential. This is rather similar to (3.35). If the variables ω' are changing rapidly and the condition (3.29) is satisfied (Δ in this case measures the magnitude of the matrix elements of Ω), we may conclude that the asymptotic behavior of correlation functions

$$\langle \chi_j(t) \chi_k(0) \rangle = \phi_{jk}(t)$$

is determined by

$$(\phi(t)) = -\Gamma(\phi(t)) \quad (3.38)$$

where (ϕ) is the matrix $(\phi_{jk}(t))$ and Γ is the matrix given by

$$\Gamma = \int_0^\infty \langle \Omega(t) \Omega(t + \tau) \rangle d\tau \quad (3.39)$$

so that we have

$$(\phi_{jk}(t)) = e^{-\Gamma t} (\phi_{jk}(0)). \quad (3.40)$$

Thus, the decay constants of the correlation functions are the eigenvalues of Γ .

It is very interesting to note that the above argument has a very

close connection with the damping theory or Wigner-Weisskopf method of quantum-mechanics. The problem there is exactly the evaluation of (3.35) and is quite similar to our stochastic problem as we have seen in the above. The exponential decay is derived from this theory for a time t which is not too short and not too long. t must not be too long, and much shorter than the Poincare cycles in the classical language. For a time comparable to Poincare cycles, exponential decay does not apply but rather the system will behave quasi-periodically. This problem is solved by an evaluation of a pole by an adequate approximation to take care of this limitation of t . This is almost exactly the same argument that we used here for our stochastic problem. The assumption of the stochastic behavior of the frequency modulation can be interpreted as the elimination of Poincare cycles, taking the limit $V \rightarrow \infty$ (V = size of the system in consideration) and keeping t in a finite range.

To the writer, the above mentioned remark seems to be of great importance in clarifying the reason behind the irreversible behavior of nature.

3.2. Behavior of Correlation Function and Simple Approximations

- 1) An autocorrelation function of the type

$$\phi(t) = \langle \{ A(0) A(t) \} \rangle \quad (3.41)$$

is generally expected to behave as shown in Fig. 8. It starts with hori-

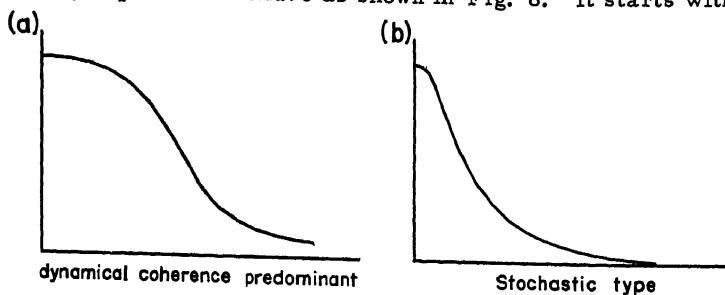


Fig. 8

zontal tangent at $t = 0$, because

$$\begin{aligned} \dot{\phi}(0) &= \langle \{ A(0) \dot{A}(0) \} \rangle = 0 \\ \ddot{\phi}(0) &= - \langle \dot{A} \dot{A} \rangle < 0 \end{aligned} \quad (3.42)$$

For a large t , $\phi(t)$ will decrease faster, with nearly an exponential decay in many favorable cases. Two typical cases are to be distinguished. The first is the case where the dynamical coherence dominates, which means that the condition (3.42) strongly keeps its influence for the important part of $\phi(t)$. The second may be called the stochastic type. This is the case where the dynamical coherence is lost at the earlier stage and decay of the type (3.40) predominates over most part. The simplest model to illustrate this situation has been provided by the Gaussian model discussed in the previous section (Eqs. (3.14), (3.17), (3.18)). For this model, the case (a) is described by $\exp(-\Delta^2 t^2/2)$ and the case (b) by $\exp[-t \tau_c \Delta^2]$. The discrimination of the two cases is roughly made by seeing whether the cross point of these two functions lies in the important region or not. The cross point is near $\gamma \sim \tau_c$ so that the condition is $\exp(-\tau_c^2 \Delta^2) \gg 1$ or $\ll 1$, which is naturally the condition (3.12), $\tau_c \Delta \gg 1$ or $\ll 1$. Now we are interested in an integral of the type

$$I = \int_0^\infty \phi(t) dt = \int_0^\infty \langle \{A(0) A(t)\} \rangle dt$$

in order to calculate the kinetic coefficients. Therefore we see that there are quite different situations in the two limits of the cases (a) and (b). In the case (a), I , or the area covered by $\phi(t)$ is determined mostly by the region of t where the dynamical coherence is important. On the other hand, it will be determined in the case (b) to a good approximation by the stochastic behavior of ϕ . The latter case (b) is more familiar to us.

Traditional treatment of setting up transport equations to calculate kinetic coefficients can only be justified if we are really in this situation. Transport equations such as the Boltzmann equation or Bloch equation are essentially approximations which can be used to calculate the correlation function or response function asymptotically for large t . The use of them is not justified if the problem corresponds to the case (a).

The transport phenomena belonging to the category (a) have not been treated in traditional theories, but we actually meet often such problems.* The so-called impurity conduction and the conduction due low mobility carriers in some semiconductors belong certainly to this category. Also the problem of spin-diffusion is of this type. Discussions of these problems are very interesting and this is just the place where our new standpoint will be most valuable.

2) In some cases of (b), a useful approximation is easily obtained for the evaluation of $I = \int_0^\infty \phi(t) dt$. The time constant of the decay of ϕ may be estimated by rewriting it in the form

* Some people call them non-Bloch problems, but the writer prefers to call them as non-Boltzmann transport problems, although he does not like to invent new words.

$$\phi(t) = \phi(0) + \int_0^t (t-\tau) \ddot{\phi}(\tau) d\tau . \quad (3.43)$$

Let us suppose that the integral

$$\int_0^{\tau_o} \ddot{\phi}(\tau) d\tau \quad (3.44)$$

has a plateau value for τ_o in the range,

$$\tau_c \ll \tau_o \ll \tau_r$$

where τ_c characterizes the time change of $\ddot{\phi}(\tau)$ and τ_r that of $\phi(t)$. Then we may write (3.43) as

$$\phi(t) = \phi(0) \left\{ 1 + t \int_0^{\tau_o} \ddot{\phi}(\tau) d\tau / \phi(0) + \dots \right\} ,$$

and find the time constant

$$\frac{1}{\tau_r} = - \int_0^{\tau_o} \ddot{\phi}(\tau) d\tau / \phi(0) . \quad (3.45)$$

This procedure is somewhat tricky, because if the integration (3.44) is carried to $\tau_o \rightarrow \infty$ we should have

$$\int_0^{\infty} \ddot{\phi}(\tau) d\tau = 0 . \quad (3.46)$$

But if τ_o is chosen appropriately (this is possible if we are really dealing with stochastic cases), (3.45) gives a useful approximation.

A simple example will perhaps help our understanding. Let us consider the expression for conductivity

$$\sigma = \frac{e^2 n}{3kT} \int_0^{\infty} \langle \vec{n}(0) \vec{n}(t) \rangle dt \quad (3.47)$$

(classical), so that we have the correlation function

$$\phi(t) = \langle \vec{v}(0) \vec{v}(t) \rangle \quad (3.48)$$

for which

$$\begin{aligned} \ddot{\phi}(t) &= \langle \vec{v}(0) \ddot{\vec{v}}(t) \rangle = -\langle \vec{v}(0) \vec{v}(t) \rangle \\ &= \langle \vec{f}(0) \vec{f}(t) \rangle / m^2. \end{aligned} \quad (3.49)$$

Thus, $\ddot{\phi}(t)$ is essentially the correlation function of the force acting on an electron. Eq. (3.45) gives, for this example,

$$\begin{aligned} \frac{1}{\tau_r} &= \int_0^{\tau_o} \frac{\langle \vec{v}(0) \vec{v}(t) \rangle dt}{\langle \vec{v}^3 \rangle} \\ &= \frac{1}{m^2} \int_0^{\tau_o} \langle \vec{f}(0) \vec{f}(t) \rangle dt / \langle \vec{v}^2 \rangle. \end{aligned} \quad (3.50)$$

The upper limit of the integral has to be finite, primarily. If $\tau_o \rightarrow \infty$, it will vanish.

Now let us suppose that the electron is scattered time to time, with the mean free time τ_f and with a short duration-time τ_d of one collision. In the limit $\tau_d \rightarrow 0$ the forces are just pulses acting on the electron when it passes the scatterers. So we assume

$$\tau_d \ll \tau_f. \quad (3.51)$$

τ_d measures the correlation time of \vec{f} and τ_f that of \vec{v} . If τ_o in (3.50) is chosen as

$$\tau_d \ll \tau_o \ll \tau_f \quad (3.52)$$

τ_r can easily be found. Namely, we have

$$\int_0^{\tau_o} \langle \vec{v}(0) \vec{v}(t) \rangle dt \approx \frac{1}{2\tau_o} \int_0^{\tau_o} dt' \int_0^{\tau_o} dt'' \langle \vec{v}(t) \vec{v}(t'') \rangle \quad (3.53)$$

$$= \frac{1}{2T_0} \cdot \frac{\gamma_0}{\gamma_f} \left\langle (\vec{v}' - \vec{v}'')^2 \right\rangle$$

where γ_0/γ_f is the probability to have a collision during T_0 , and \vec{v}' and \vec{v}'' are the initial and final velocities of a collision. Eq. (3.53) gives

$$\begin{aligned} \frac{1}{\tau_r} &= \frac{1}{\langle \vec{v}^2 \rangle} \cdot \frac{1}{2\gamma_f} \left\langle \vec{v}'^2 - 2\vec{v}'\vec{v}'' + \vec{v}''^2 \right\rangle \\ &= \frac{1}{\tau_f} (1 - \langle \cos \theta \rangle) \end{aligned}$$

with

$$\langle \cos \theta \rangle = \langle \vec{v}' \cdot \vec{v}'' \rangle / \langle \vec{v}^2 \rangle \quad (3.54)$$

the average of the cosine of the scattering angle. Eq. (3.54) is the well-known formula for the relaxation time.

For this particular model, we may easily calculate $\phi(t)$ explicitly. Let us define the transition probability of the jump from \vec{v} to \vec{v}' by $\Phi(\vec{v}, \vec{v}')$ and write

$$k g(\vec{v}) \equiv \int \Phi(\vec{v}, \vec{v}') d\vec{v}' g(\vec{v}')$$

Then we find easily that

$$\int_0^\infty e^{-st} \left\langle \vec{v}(0) \vec{v}(t) \right\rangle dt = \gamma_f \int f_0(\vec{v}) d\vec{v} \cdot \left(\vec{v} - \frac{1}{1+s\gamma_f-k} \vec{v} \right) \quad (3.55)$$

where $f_0(\vec{v})$ is the equilibrium distribution of \vec{v} . This is a general expression. If the scattering is assumed to be elastic, (3.55) reduces to

$$\int_0^\infty e^{-st} \phi(t) dt = \frac{\gamma_r}{1+s\gamma_r} \left\langle \vec{v}^2 \right\rangle \quad (3.56)$$

and so

$$\phi(t) = \left\langle \vec{v}^2 \right\rangle e^{-t/\gamma_r} \quad (3.57)$$

and

$$-\ddot{\phi}(t) = \frac{\langle \vec{v}^2 \rangle}{\tau_r} \left\{ \delta(t) - \frac{1}{\tau_r} e^{-t/\tau_r} \right\}. \quad (3.58)$$

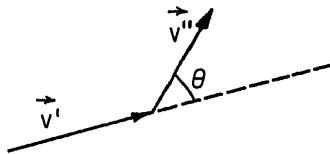


Fig. 9

Thus the correlation function of the force, (3.49) behaves like that shown in Fig. 10. So long as τ_d is very small compared to τ_f , (3.50) may be regarded to have such a plateau value.

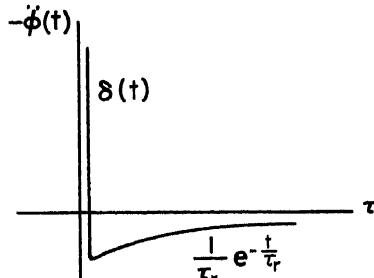


Fig. 10

3) Now we come back to (3.45), or

$$\frac{1}{\tau_r} = \int_0^{\tau_0} \langle \dot{A}(0) \dot{A}(t) \rangle dt / \langle \dot{A}^2 \rangle. \quad (3.59)$$

This equation is quite similar to (3.28) for motional narrowing and has really the same character, except that the simple decay of $\phi(t)$ is not guaranteed and hence τ_r as given (3.59) is only a rough measure for the asymptotic time constant of $\phi(t)$.

But, if the situation is such that a simple exponential decay of $\phi(t)$ is a good approximation, then we shall have:

$$\int_0^\infty \langle A(0) A(t) dt \sim \frac{\langle A^2(0) \rangle}{\int_0^{\tau_o} \langle \dot{A}(0) \dot{A}(t) \rangle dt} \quad (3.60)$$

by assuming $\exp(-t/\tau_r) = \phi(t)$. Eq. (3.60) becomes exact if the spectrum of relaxation time is degenerate. If a perturbation calculation is used (which is not always permissible), τ_o may often be put equal to infinity, because the perturbation calculation starts by treating each scattering process as independent.

Kirkwood's formulas for the friction constant of a Brownian particle¹⁸ is just Eq. (3.60) giving the friction constant in terms of the correlation of the force acting on it. We may apply Eq. (3.60) for the calculation of electronic conductivity assuming phonon scattering. Then we shall obtain the famous Gruneisen formula as the first approximation.³⁰

Similar applications can be made to magnetic resonance problems. Kubo and Tomita's paper deals with this problem, including the problem of motional narrowing.¹⁹

3.3. Discussion of Traditional Transport Equations

1) Finally we shall discuss a little more the traditional method of using transport equations from our point of view. Let us take the example of electric conduction. The customary equation of transport has the form

$$\frac{\partial f}{\partial t} + \vec{v} \cdot \frac{\partial f}{\partial \vec{r}} + \vec{v} \cdot \frac{\partial f}{\partial \vec{p}} = \Gamma(f) \quad (3.61)$$

where $f(\vec{p}, \vec{r})$ is the one-electron distribution function usually and $\Gamma(f)$ is the collision operator. So $\Gamma(f_e) = 0$ for equilibrium distribution f_e . For simplicity, let us assume that the system is spacially homogenous so that the second term on the left hand side will be omitted. We write

$$f = f_e + g$$

and

$$\Gamma(f_e + g) = -Dg \quad (3.62)$$

by assuming also

$$g \ll f_e$$

Then we get a linearized equation from (3.61)

$$\frac{\partial g}{\partial t} - \frac{eE}{m} \frac{\partial f_0}{\partial \vec{n}} = -Dg \quad (3.63)$$

the solution of which is

$$g(t) = \int_{-\infty}^t e^{-D(t-t')} \frac{e\vec{E}(t')}{m} \cdot \frac{\partial f_0}{\partial \vec{n}} dt', \quad (3.64)$$

thus the current is given by

$$\vec{j}(t) = \int d\vec{n} \cdot e\vec{n} \int_{-\infty}^t \left(e^{-D(t-t')} \frac{\partial f_0}{\partial \vec{n}} \right) \frac{e\vec{E}(t')}{m} dt'$$

which may also be written as

$$\vec{j}(t) = \frac{ne^2}{kT} \int_{-\infty}^t dt' \int f_0(\vec{n} e^{-D(t-t')} \vec{n}) d\vec{n} \cdot \vec{E}(t') dt'. \quad (3.65)$$

Therefore the conductivity is

$$\sigma = \frac{ne^2}{kT} \int_0^\infty \langle \vec{n} e^{-Dt} \vec{n} \rangle dt = \frac{ne^2}{kT} \int_0^\infty \langle \vec{n} \vec{n}(t) \rangle dt.$$

This is just to show that ordinary transport equation leads to the same expression for the conductivity in a less general way.

Conversely, the original expression of conductivity (2.55) or (2.66) allows an elementary interpretation. Let us assume for simplicity that the density matrix and the current are diagonal in the momentum \vec{p} . Then (disregarding the statistics) we may write³¹

$$\begin{aligned} & \text{Tr } \rho j(0) j(t) \\ &= \sum_p \sum_{p'} \rho(p) \left| \langle p | e^{iHt/\hbar} | p' \rangle \right|^2 j(p) j(p') \end{aligned} \quad (3.67)$$

$$= \sum \sum \rho(P) W(P \rightarrow P'; t) j(P) j(P') .$$

Here the transition probability $W(P \rightarrow P'; t)$ is defined by

$$W(P \rightarrow P'; t) = |\langle P | e^{iHt/\hbar} | P' \rangle|^2 . \quad (3.68)$$

Then the problem is just to find $W(P \rightarrow P'; t)$ or to find an equation which it satisfies if such an equation exists.

2) We discussed in the above the simple case of independent particles. More generally we may treat the whole system in quite a similar way. The probabilistic equation for the whole is called the master equation.

We started in Part 2 from the dynamical equations for the whole system to obtain (2.8) or (2.14). As far as the dynamical disturbance is concerned, these solutions are correct in the first order, irrespective of the size of the system. The system may be small and the response function may not decay at all but continue to oscillate. Still the general expression of admittance itself is correct. In this sense, the general theory may include irreversible processes, but it has not exhibited the most essential point of irreversible processes. That is how one can derive the irreversible behavior of a macroscopic system from the dynamical equations. I am not prepared to spend time in this deep problem but will point out only that the correlation functions or response functions will be shown to decrease asymptotically as t grows.

For this we have to make the size V of the system* grow to infinity before we make t large. This corresponds to elimination of Poincare cycles.

It is also to be remembered that the same consideration is always made for the scattering problem in quantum mechanics.

3) It is therefore possible to use the Wigner-Weisskopf method for a formal treatment of our problem. It can be generalized to apply to the density matrix itself rather than the wave function. Namely, the solution of the equation of motion of density matrix

$$\frac{\partial \rho}{\partial t} = \frac{1}{i\hbar} [H, \rho] = \frac{1}{i\hbar} H^x \rho \quad (3.69)$$

can be written as

$$\rho(t) = \frac{1}{2\pi i} \int_{-\infty}^{+\infty} \frac{e^{st}}{S + \frac{1}{i\hbar} H^x} \rho(0) . \quad (3.70)$$

* The number of particles will usually increase with V .

The problem is now to evaluate this for t in a certain range when the Hamiltonian has the structure

$$H = H_0 + H' \quad H'^X = H_0^X + H'^{X'} \quad . \quad (3.71)$$

Although the original Wigner-Weisskopf method applies to $(s - H/i\hbar)^{-1}$ rather than $(s + H'/i\hbar)^{-1}$ we may apply it to (3.70) with appropriate modification to determine approximate pole of s to evaluate (3.70) in an asymptotic way. This has, again, as we pointed out before, a close connection with the concept of motional narrowing.

For example, let us consider a system A coupled with a big system B, which we call the reservoir. A is perturbed by the interaction H' with B. Now the equation of motion of the density matrix for the system as a whole is transformed into

$$\frac{\partial \bar{\rho}}{\partial t} = \frac{1}{i\hbar} [H'(t), \bar{\rho}] \equiv \frac{1}{i\hbar} H'(t)^X \bar{\rho} \quad (3.72)$$

by the transformation

$$\rho = e^{i(H_A + H_B)t/\hbar} \bar{\rho} e^{-i(H_A + H_B)t/\hbar} \quad . \quad (3.73)$$

Eq. (3.72) is a close analogy to (3.23) or (3.36) if $H'(t)$ is considered as a stochastic variable. In order to secure this analogy, we assume $\bar{\rho}$ to be expressed by

$$\bar{\rho} = \bar{\rho}_A \times \rho_B^\circ \quad (3.74)$$

where ρ_B° is an equilibrium density matrix for B, and take the average on this. The crudest approximation corresponding to the limit of motional narrowing gives

$$\frac{\partial \bar{\rho}_A}{\partial t} = -\Gamma \bar{\rho}_A \quad (3.75)$$

or

$$\frac{\partial \rho_A}{\partial t} = \frac{1}{i\hbar} [H_A, \rho_A] - \Gamma \rho_A \quad (3.76)$$

where

$$\Gamma \rho_A \equiv \frac{1}{\hbar^2} \int_0^\infty dt \langle [H'(t) [H'(0), \rho_A]] \rangle_B \quad (3.77)$$

determines the asymptotic behavior of $\rho_A(t)$. This approximation is exactly the one that one obtains in the second order perturbation theory. Eq. (3.77) includes both the self-energy correction and the usual transition probability. Eq. (3.76) is the same equation as used by Bloch in his general theory of the magnetic relaxation problem.³² The assumption involved here is that $H'(t)$ changes very rapidly as the result of the natural motion of B and further H' itself is small enough. This condition allows us to apply this approach for large t , which is the order of

$$1/t \sim (|H'|^2/\hbar^2) \times \tau_c ,$$

τ_c being the correlation time of $H'(t)$. This condition is essentially of the same nature as that which Van Hove proved.²⁹

It is a very basic and also very difficult problem to examine more exactly the logic by which one arrives at the transport equations starting from the dynamical equations, either classical or quantum-mechanical. A famous contribution was made by Bogolubov³³ in which he tried to derive classical transport equation of gas by classical dynamics. Van Hove's formulation of perturbation theory is also to be highly appreciated. More recently, Luttinger and Kohn investigated the problem particularly for electron systems.³⁴

Generally speaking, the traditional transport equations will be justified in two cases. One is the case where the perturbation is always weak, and the other is the case where the perturbation is very local. For example, the phonon scattering of electrons may be considered to belong to the first category. At least one can think of the limit of very weak electron-phonon scattering and justify the use of customary perturbational calculation. Van Hove's theory can be applied to this case. The second case corresponds to impurity scattering. The interaction of impurity and electron may be strong, but it should be assumed to have rather short force range so that the condition (3.51) $\gamma_d \ll \gamma_f$ is satisfied. This case has been analysed in great detail by Kohn and Luttinger (1958). These theories have many things in common with the various methods employed for the analysis of multiple scattering and many body problems. It is hoped that the recent developments in these fields will aid each other.

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MULTIPLE PRODUCTION OF MESONS AND A NONLOCAL THEORY OF FIELDS*

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I. Introduction

The idea of a nonlocal field theory or of a theory of interactions limited by a universal relativistic cut-off operator arose from the study of the fundamental divergence difficulties encountered in the theory of point-interactions between point-particles.

Today direct experiments show that the "physical particles," like protons and neutrons, have complex structures, and their quantum statistical description makes use of the concept of nonlocalized interactions or nonlocalized distributions of charges and magnetic moments.

M. A. Marcow and H. Yukawa¹⁹ suggested that the operators representing the field amplitudes could be "nonlocal," e. g., in a representation in which x are diagonal, these operators could be represented only by non-diagonal matrices $\langle x'|\psi|x''\rangle$, not reducible to the form:

$$1 \quad f(x') \delta^4(x' - x'').$$

Such fields would not commute with each other. This non-local character of fields follows also from the method of "relativistic cut-off" discussed below. A great deal about such nonlocal interactions can be learned from experiments in high energy collisions. In the following I shall refer mostly to collisions of particles which in the centre of momenta frame have $E \geq 10^9$ ev. Observations on cosmic rays give us remarkable indications that our ability to explore small space-time domains by the use of these particles is limited in a very peculiar way. One can expect the existence of a supplementary uncertainty in measurements of distances and time intervals within small domains, D_t . Under certain conditions the linear extension of these domains is comparable to the Compton wavelength of a nucleon, $l = \frac{\hbar}{Mc} \sim 2 \cdot 10^{-14}$ cm. It is important to note that the existence of such 4-dimensional domains of uncertainty does not limit the validity of the homogeneous Lorentz transformation in the momentum space (p-space).

In the following, strict validity of the homogeneous Lorentz transformation in the momentum variables and of the conservation of the total energy-momentum 4-vector will be assumed, as well as the validity of:

- 1) the conservation law of the electric charge;

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- 2) conservation of the baryon number;
 3) conservation of the total angular momentum.

We shall begin with the study of some problems regarding the cosmic ray "jets" and report briefly on models proposed by Heisenberg, Fermi, and Landau in order to understand better these remarkable phenomena. At the end I shall outline the approach to the theory of high energy collisions I suggested some time ago, deriving it from a nonlocal field theory, and shall compare it with experimental data.

Most of the theoretical consideration will be made with reference to the center of momentum system (CM) of the colliding particles, because this choice not only simplifies the calculations but also reveals the fundamental importance of the CM system in separating space and time. Indeed, from observations on several hundred jets, one can deduce that a jet in the CM system of the colliding particles exhibits very remarkable symmetries. Moreover, in a nonlocal theory of fields, the momentum distribution in the CM frame is connected with some fundamental statistical properties of space and time and of the phase-space.

From the field theoretical viewpoint, the most interesting cases are found in "jets" defined as high energy collisions between two nucleons or between one meson and one nucleon. Such "jets" are usually composed of a dense narrow core of relativistic particles surrounded by tracks making less acute angles with the direction of the primary. The "jets" were observed many years ago in cloud chambers and in nuclear emulsions. A jet is composed mostly of pions and nucleons, but eventually can contain also K mesons, as well as baryons and antibaryons. Sometimes (if the inspection of emulsions at distances of several radiation units is possible) electron showers generated by γ rays from π^0 decays are also observed.

Let us limit ourselves to the analysis of nucleon-nucleon collisions in which n mesons (n "relativistic" shower particles) are created. n is called the multiplicity of the shower. We denote the momentum 4-vectors of the incident particles by $p_{1\mu}^{(i)}$, $p_{2\mu}^{(i)}$ and their final momenta by $p_{1\mu}^{(f)}$, $p_{2\mu}^{(f)}$. The total momentum of the system is denoted by P_μ and the individual momenta of the created n shower particles by $K_{1\mu}, K_{2\mu}, \dots, K_{n\mu}$ where $\mu = 0, 1, 2, 3$. The metric tensor is taken to be: $g_{00} = 1$; $= -g_{11} = -g_{22} = -g_{33}$, and natural units ($\hbar = 1$, $c = 1$) will be used in nearly all cases. The conservation of energy and momentum states:

$$P_\mu = p_{1\mu}^{(i)} + p_{2\mu}^{(i)} = p_{1\mu}^{(f)} + p_{2\mu}^{(f)} + K_{1\mu} + \dots + K_{n\mu} \quad (1)$$

$$(\mu = 0, 1, 2, 3).$$

In the case of a nucleon-antinucleon, annihilation:

$$p_{1\mu}^{(f)} = p_{2\mu}^{(f)} = 0.$$

The center of momentum system is defined by

$$O = \bar{P} = \vec{p}_1^{(l)} + \vec{p}_2^{(l)} = \vec{p}_1^{(f)} + \vec{p}_2^{(f)} + \bar{K}_1 + \dots + \bar{K}_n. \quad (1')$$

It is evident that the total energy, P_0 , is minimum in the CM system. We also define the coefficient of inelasticity, K , as:

$$K = \left(\frac{\epsilon_1 + \epsilon_2 + \dots + \epsilon_n}{E_1^{(l)} + E_2^{(l)}} \right)_{CM} = 1 - \left(\frac{p_{1o}^{(f)} + p_{2o}^{(f)}}{p_{1o}^{(i)} + p_{2o}^{(i)}} \right)_{CM} \quad (2)$$

where $\epsilon_r = K_{ro} = \sqrt{m_r^2 + \vec{K}_r^2}$ are the energies of the created particles. $E_1^{(l)}, E_2^{(l)}$ are the initial energies of the nucleons. The definition of K is unambiguous only if we know the final states of the incident nucleons, or if we can distinguish between created particles and the final states of the incident nucleons. Obviously, in an annihilation process, $K = 1$. Assuming that $P_\mu P^\mu = m^2 > 0$, we introduce the following 4-vector

$$U_\mu = \frac{1}{m} P_\mu. \quad (3)$$

One has $U_\mu U^\mu = 1$ and, in the CM system, the components of U_μ are $(1, 0, 0, 0)$. The energy component in the CM system $(K_0)_{CM}$ of an arbitrary 4-vector K_μ can be written clearly in the following invariant form: $(K_0)_{CM} = K_{\mu\nu} U^\mu$.

Thus, the definition (2) can be put in the invariant form:

$$K = \frac{\sum_{r=1}^n K_{r\nu} U^\nu}{P_\mu U^\mu}. \quad (2')$$

If the relation,

$$[\vec{p}_1^{(f)} + \vec{p}_2^{(f)}]_{CM} = O,$$

is satisfied in the CM system (hence $(\sum_{r=1}^n \bar{K}_r)_{CM} = O$), K takes the same functional form, exhibited in Eq. (2), without the subscript CM, in any frame of reference.

II. Momentum Distribution in Jets

Let us briefly describe how one obtains from the measurements of angles and momenta of the created particles of a jet the distribution of the momenta in the CM system, the values of the energy of the incident particle, and the inelasticity parameter, K. Since usually only the angles are easily measurable, whereas the values of the momenta are known only with great uncertainty, and since usually some of the created neutral particles are not observed, one needs to apply an approximate treatment based on a few plausible assumptions about the structure of the jet.

The distribution of the relativistic trajectories observed in jets of high energy shows in the emulsions ("laboratory reference frame" L) the following structure (see Figs. 1 and 2): a narrow cone which contains nearly half the total number of tracks. The other half forms a wider cone. The narrow cone in some typical case can have an aperture $\sim 10^{-4}$ rad., whereas the wide cone has angles $\sim 10^{-2}$ rad. In low energy jets, for example, in one formed in a p-p collision in the 9 Bev proton beam of the Synchrophasotron at Dubna, the wide cone containing 8 particles has an aperture of ~ 0.3 rad.¹

In order to become familiar with the analysis of the angular and momentum distributions in jets, it will be useful to recall a few elementary formulae of relativistic kinematics.

Let us consider the collision of two particles having masses M_1 and M_2 respectively:

$$M_1^2 = \bar{p}_{1\mu}^{(i)} p_{1\mu}^{(i)\mu} ; \quad M_2^2 = \bar{p}_{2\mu}^{(i)} p_{2\mu}^{(i)\mu}$$

and let us assume that in the laboratory frame L the particle M_2 is at rest: $\bar{p}_2^{(i)} = 0$. Let us choose the direction of $\bar{p}_1^{(i)}$ of the incident particle in L as the direction of the x_1 axis and let us denote by \bar{p}_y the components in the CM system of an arbitrary 4-vector with components p_y in the L-system. Then the special Lorentz transformation connecting the two systems can be written:

$$p' = \gamma_c (\bar{p}' + \beta_c \bar{p}^\circ) .$$

$$p^2 = \bar{p}^2 \quad p^3 = \bar{p}^3$$

$$p^\circ = \gamma_c (\bar{p}^\circ + \beta_c \bar{p}')$$

where β_c is the velocity of the CM system relative to the L system and $\gamma_c = (1 - \beta_c^2)^{-1/2}$.

Indicating by ϑ and θ the polar angles in the CM frame and in

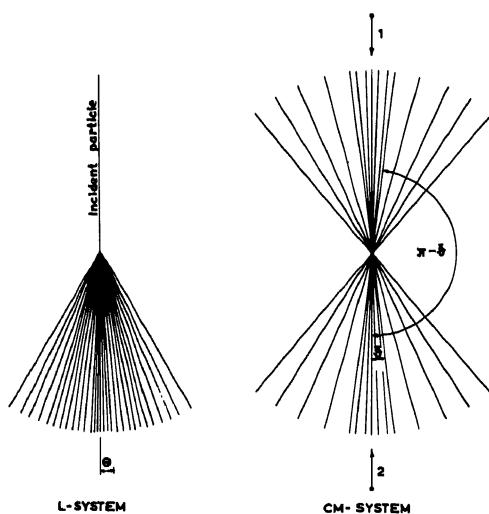


Fig. 1

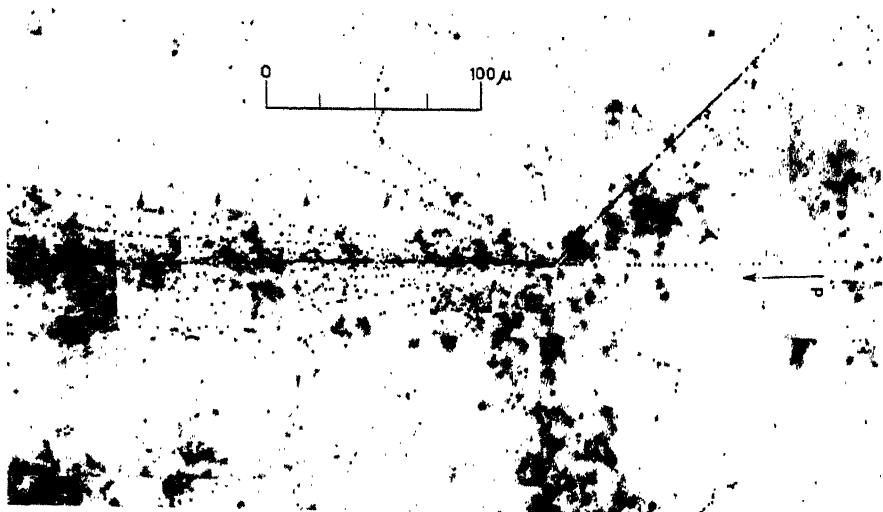


Fig. 2 Turin Jet

the L frame respectively which a momentum-vector \vec{p} forms with the axis of x_1 (or of p_1), we have:

$$\bar{p}_1 = |\vec{p}| \cos \theta, \quad \bar{p} = \sqrt{\bar{p}_1^2 + \bar{p}_2^2 + \bar{p}_3^2} \cos \bar{\vartheta}, \text{ etc.}$$

and remembering that

$$\frac{\bar{p}_1}{|\vec{p}|} = \frac{1}{\beta} \quad ; \quad \frac{\bar{p}}{\sqrt{\bar{p}_1^2 + \bar{p}_2^2 + \bar{p}_3^2}} = \frac{1}{\beta},$$

we obtain (by putting $\bar{p}_3 = 0$; $\bar{p}_2/\bar{p}_1 = \tan \theta$)

$$\tan \theta = \frac{1}{\gamma_c} \frac{\sin \bar{\vartheta}}{\cos \bar{\vartheta} + \beta_c/\beta}, \quad (4)$$

which is the well known formula used extensively in the analysis of jets.

Experimentally one finds that the momentum distribution of the created charged mesons in most cases is symmetric with respect to the plane perpendicular to the axis of the jet. Such a symmetry is to be expected in the cases of proton-proton and of neutron-neutron collisions. But in cases of pion-nucleon, proton-neutron, or baryon-antibaryon collisions such symmetry cannot be postulated. Usually, in the analysis of jets, one assumes the validity (at least approximate) of this symmetry as an experimentally established property of jets.

Then, indicating by $\bar{\vartheta}_f$ and $\bar{\vartheta}_b = \pi - \bar{\vartheta}_f$ the angles formed in the CM system by two symmetrically oriented particles in the forward cone

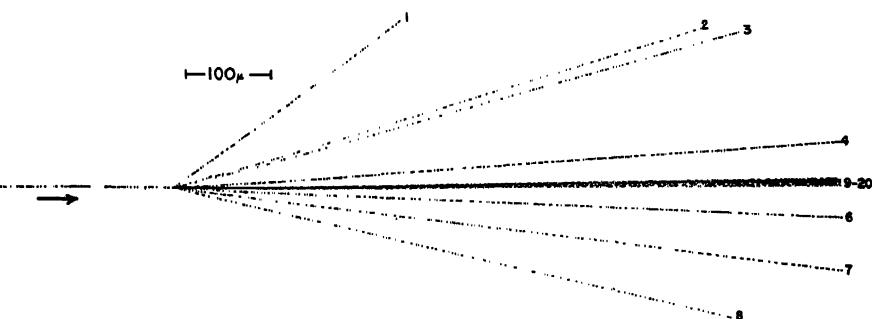


Fig. 3 A beautiful illustration of a typical high energy jet.
(Courtesy Marcel Schein, University of Chicago.)

and in the backward cone respectively, and indicating by θ_f and θ_b the corresponding laboratory angles, one obtains from Eq. (4),

$$\gamma_c^2 \tan \theta_f \tan \theta_b = - \frac{\sin^2 \bar{\vartheta}_f}{(\beta_c/\bar{\beta})^2 - \cos^2 \bar{\vartheta}_f}. \quad (5)$$

In high energy events one can assume with good approximation that $\beta_c \sim 1$ and $\bar{\beta} \sim 1$ and thus $\beta_c/\bar{\beta} = 1$. With this approximation Eq. (4) becomes:

$$\gamma_c \tan \theta = \tan \frac{\bar{\vartheta}}{2}. \quad (4')$$

The right-hand side of Eq. (5) is then equal to unity. Taking the logarithm of Eq. (5) and summing over all n particles of the jet, one gets:

$$n \log \gamma_c + \sum_{r=1}^n \log \tan \theta_r = 0. \quad (5')$$

From this relation and from the measurements of all θ_r , one obtains the value of the parameter $\gamma_c = (1 - \beta_c^2)^{-1/2}$ of the CM reference frame.²

Let us call the angle θ_m in the L-system corresponding to $\bar{\vartheta}_f = \bar{\vartheta}_b = \pi/2$ the median angle of the jet. Obviously,

$$\gamma_c = \frac{1}{\tan \theta_m} \quad \text{and} \quad \gamma_c \sim \frac{1}{\theta_m} \quad \text{if} \quad \theta_m \ll 1.$$

As usual, θ_m is small, [$\theta_m \lesssim 10^{-2}$]. This relation gives another simple possibility of measuring γ_c . This method was used extensively in the early work on jets. The Bristol group proposed displaying the angular distribution graphically by plotting the values of $\log \tan \theta_r$ ($r = 1, \dots, n$) on an axis, as in Fig. 4.³ The points representing tracks in the forward and in the backward cones appear distributed symmetrically with respect to the point representing the median angle θ_m since from Eq. (4')

$$\log \tan \theta_r - \log \tan \theta_m = \log \tan \frac{\bar{\vartheta}_r}{2}$$

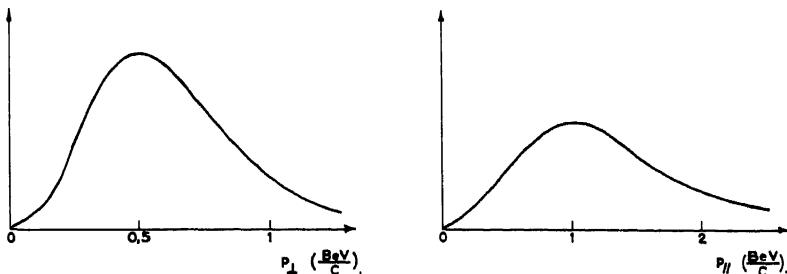


Fig. 4

so that the points corresponding to $\overline{\vartheta}_r = \overline{\vartheta}_f$ and to $\overline{\vartheta}_r = \pi - \overline{\vartheta}_f = \overline{\vartheta}_b$ appear equidistant from the point representing the median angle (as is obvious also from an inspection of Eq. (5)). It is noteworthy that the majority of jets display such a symmetry. Exceptions are reducible in many cases to "plural" collision processes: if a nucleon hits a heavy nucleus, it is possible that after a first collision with one nucleon of the target-nucleus the primary nucleon or some secondary particle makes some other collision with a nucleon of the same target-nucleus. Such "plural" collision processes are frequently observed and need a special theoretical treatment. But this question will not be considered here.

If one knows the masses M_1 and M_2 of the colliding particles, the knowledge of the parameter γ_c allows one immediately to find the energy $E_i^{(i)}$ of the incident particle. The simplest case is of the nucleon-nucleon collision in which $M_1 = M_2 = M$ (where M is the mass of a proton). Then an elementary calculation shows that, if M_2 is at rest in the L frame

$$E_1^{(i)} + E_2^{(i)} = \gamma_c (\bar{E}_1 + \bar{E}_2)_{CM} = 2 \gamma_c^2 M \quad (6)$$

because $\bar{E}_1 = \bar{E}_2 = \gamma_c M$. Thus, the primary nucleon has an energy

$$E_1^{(i)} = (2 \gamma_c^2 - 1) M. \quad (6')$$

The more general formula, for $M_1 \neq M_2$, valid if M_2 is at rest in L frame, gives the following relation between $E_1^{(i)}$ and γ_c :

$$E_1^{(i)} + E_2^{(i)} = E_1^{(i)} + M_2 = \gamma_c^2 M_2 + \gamma_c^2 \left[M_2^2 + \frac{M_1^2 - M_2^2}{\gamma_c^2} \right]^{\frac{1}{2}}. \quad (6'')$$

If $\gamma_c \gg 1$, $M_1 \approx M_2$ and $M_2 = M$, the value given by Eq. (6) constitutes a good approximation to that by Eq. (6'').

The inelasticity parameter, K , can be calculated from Eq. (2)..

in cases where the spatial momenta $|\vec{K}_1| \dots |\vec{K}_n|$ are known, e. g., the "Turin jet,"⁴ by making an assumption about the masses of the created particles, (e. g. that all created particles are pions). The value of K ($K \sim 0, 7$ in the case of the Turin jet) even in these fortunate cases, is known only roughly, because the contribution of neutral particles cannot be measured exactly.

There are several approximate methods for evaluating inelasticity. All of them give a rough order of magnitude of K . I shall not describe them, and shall only mention some results. For example, one finds $K \sim 1$ for small jets ($E_1^{(\prime)} < 10$ Bev) and $0.1 \lesssim K \lesssim 0.5$ for jets of high energy ($E_1^{(\prime)} \gtrsim 10^3$ Bev).

The angular distribution in the CM frame and the momentum spectrum are very important. Here, also, I shall mention only one of the methods used to find the angular distribution in the CM frame.

Let us consider in the CM system a cone of aperture $\bar{\vartheta}$ having as axis the axis of the jet ($\bar{\vartheta}$ being the polar angle with respect to the forward direction of the incident primary particle). For each value of $\bar{\vartheta}$ one can find the fraction $F = n'(\bar{\vartheta})/n$ of the n outgoing created charged particles whose trajectories lie inside this cone (their number is indicated by $n'(\bar{\vartheta})$). If the distribution in the CM system is isotropic, then the average number of tracks, whose directions lie inside a solid angle $\Omega = 2\pi(1 - \cos \bar{\vartheta})$ is proportional to Ω . Thus in the case of an isotropic distribution, the expectation value of F is:

$$\langle F \rangle = \frac{2\pi(1 - \cos \bar{\vartheta})}{4\pi} = \sin^2 \frac{\bar{\vartheta}}{2}. \quad (7)$$

Assuming in Eq. (4) $\beta_c/\bar{\beta} = 1$ (this assumption being a very good approximation for high energy jets) one can transform the above relation in terms of the laboratory angle θ into the equivalent (because of Eq. (4')) relation:

$$\frac{\langle F \rangle}{1 - \langle F \rangle} = (\gamma_c \tan \theta)^2. \quad (8)$$

Since $n'(\bar{\vartheta}) = n'(\theta)$ is also the number of tracks lying inside the laboratory angle θ , one easily finds the observed value of F corresponding to any prescribed values of θ . Evidently, if one plots the observed values of $\log F/(1 - F)$ as a function of $\log \tan \theta$, one finds in the case of isotropic distribution in the CM system that the experimental points will be distributed along a straight line with a slope = 2. The experimental data do not always give such a simple graphical representation, indicating a possible anisotropy. Assuming an anisotropic distribution in the CM frame of the type

$$dn'(\bar{\vartheta}) = -A' \cos^m \bar{\vartheta} d(\cos \bar{\vartheta}) \quad (9)$$

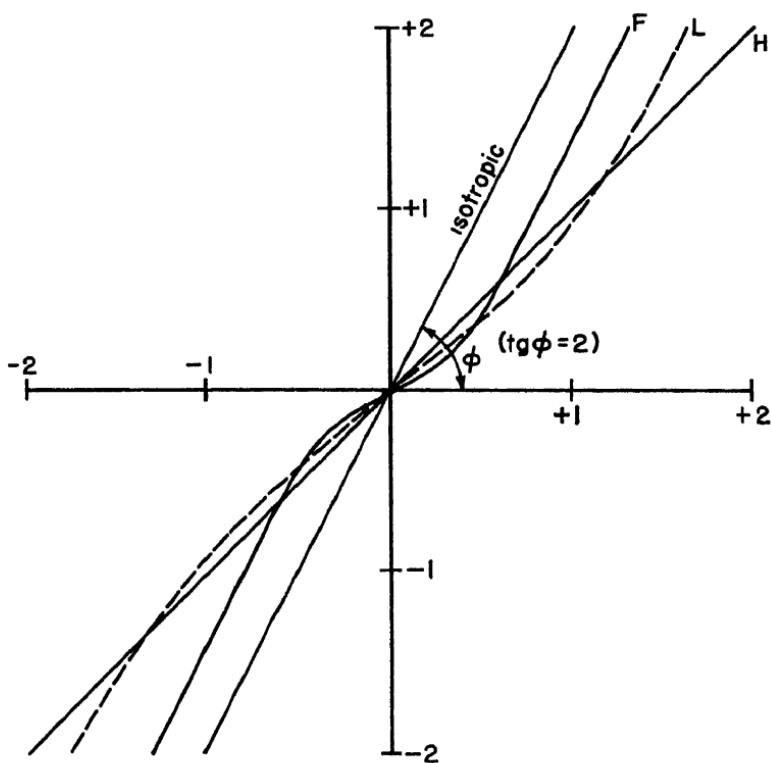


Fig. 5

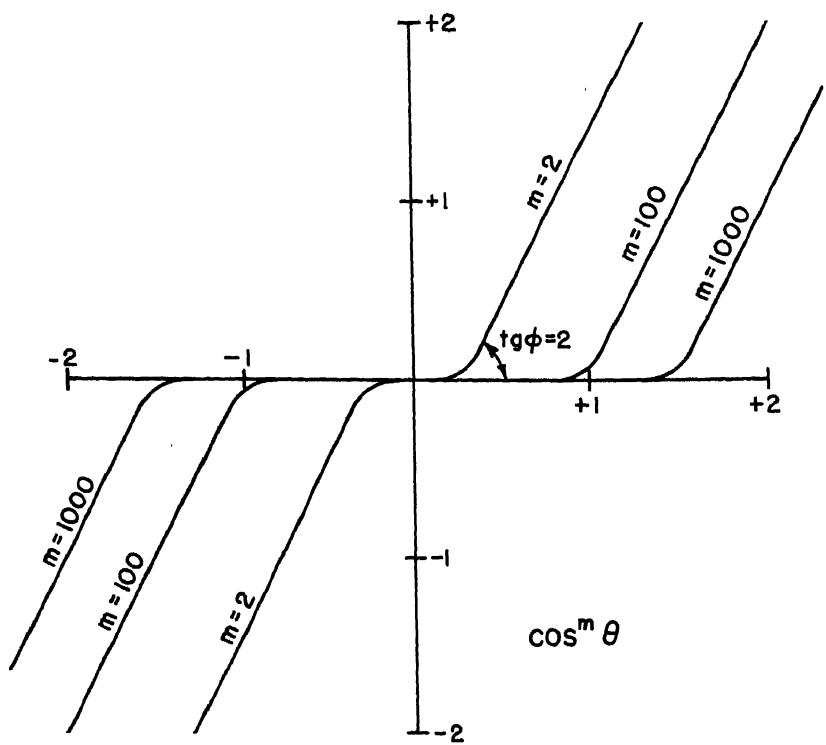


Fig. 6

with m even, one has, plotting $\log F/(1-F)$ against $\log \tan \theta$, a curve of the form indicated in Fig. 6 instead of a straight line.

The models of multiple production suggested by Heisenberg, by Fermi and by Landau give rise to angular distributions corresponding to the curves H, F, L of Fig. 5.

Experimental data show large fluctuations in m with cases of isotropy in the CM frame prevailing in the region of low total energy ($E_1^{(0)} \lesssim 10$ Bev), and with cases of sharp anisotropy occurring in high energy jets ($E_1^{(0)} \gtrsim 10^3$ Bev), corresponding to large values of the exponent m in Eq. (7).

Recently a new "2 center model" was discussed by Tagaki and by many other authors.⁵ In this model it is assumed that after the collision, two highly excited "centers" are moving in the CM system in opposite directions and are emitting secondary particles isotropically in the respective rest frames with fixed spectral distributions of momenta.

It is clear that in the 2 center model we have more parameters at our disposal and it is possible to choose them in a way so as to fit the experimental data better. The analysis of this model lies outside the scope of these lectures.

The question of the momentum spectrum of the created particles is of fundamental importance for the theory of multiple production and is, of course, connected with questions regarding the multiplicity, the inelasticity and the angular distribution.

The data concerning the neutral and the charged pions and K mesons are in agreement with the assumption that the distribution is charge independent (within the large limits of experimental errors).

Measurement of momenta and energies of the relativistic particles in jets is difficult. Therefore knowledge of the spectral distribution of momenta is rather poor.

The best established measurements concern the average transverse momentum, $\langle p_1 \rangle$, the average value of the components of $\vec{p}^{(r)}$ and of \vec{K}_r , $r=1 \dots n$ perpendicular to the axis of the jet. This component has the same value in the L reference frame and in the CM frame.

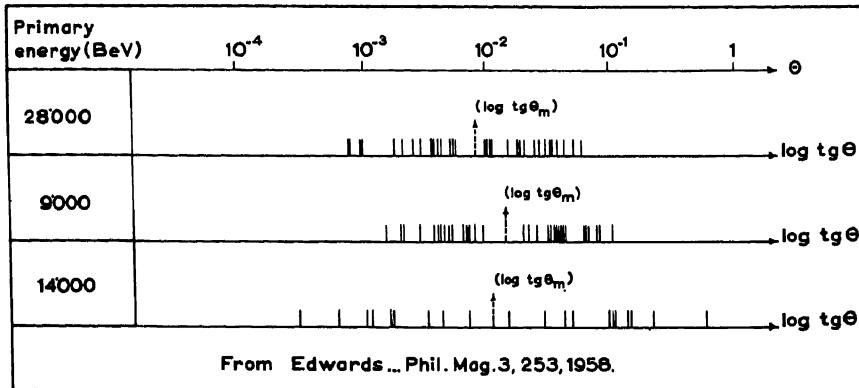
The results⁵ concerning jets of a wide range of energy (from 10^2 until 10^6 Bev) give consistently $\langle p_1 \rangle = 0.4$ Bev. $\langle p_1 \rangle$ is ~ 0.2 Bev for low energy jets ($E_1^{(0)} < 10$ Bev). In the Turin jet the average value of p_1 is = 0.4 Bev.

The spectral distribution of momenta in anisotropic, high energy jets can be given separately for the transverse components K_1 and for the longitudinal components K_z in the CM system. The observed distributions are of the types represented in Fig. 4.⁶ The average values of the momenta of nucleons are greater (of the order of 1 Bev or 2 Bev). The above spectral distributions are roughly in accord with the theoretical prediction based on the Heisenberg model of multiple production. They are also in accord with the prediction of the nonlocal theory, as will be shown below.

The experimental results can be summarized in the following

table in which we distinguish the I-group of low energy jets having nearly isotropic distribution in the CM frame, and the II-group of high energy jets, with a strongly anisotropic distribution in the CM system.

Table I



From Edwards... Phil. Mag. 3, 253, 1958.

III. The Statistical Model

It is useful to compare the experimental data on jets with the prediction of the so-called statistical theory of multiple production. I shall formulate this theory, following in some points the simple way suggested in a recent paper by P. P. Srivastava and G. Sudarshan.⁷ The statistical model was applied by Fermi to the cases of jets of low total energy. It was also considered by other authors.⁷

The main idea of this model is based on the following fundamental assumption of the quantum theory of fields: every non-degenerate (stationary) eigenstate of energy of a free particle has a statistical weight = 1. Introducing the phase-space representation, one can say that to every stationary, non-degenerated state there corresponds a cell of the phase space of volume = \hbar^3 .

In order to describe a process of multiple production (a "jet"), we shall use the S-matrix formalism. Let us denote by

$$\langle K_1 \dots K_n | p_1^{(f)} p_2^{(f)} | M | p_1^{(i)} p_2^{(i)} \rangle$$

the invariant matrix element of the S matrix which includes contributions from all possible transitions connecting a given initial state of two nucleons with a given final state of mesons and nucleons, where all these states are eigenstates of the momentum and the energy.

Let

$$f = \sum | \langle K_1 \dots K_n | p_1^{(f)} p_2^{(f)} | M | p_1^{(i)} p_2^{(i)} \rangle |^2 \quad (10)$$

be the average over initial spins and sum over the final spins of the square of the absolute value of the matrix element of the S matrix. Then the relative transition probability for the production of n mesons (as well as the cross-section σ_n) is proportional to

$$W_n = A \int d^4 p_1^{(f)} d^4 p_2^{(f)} d^4 K_1 \dots d^4 K_n S^2(K_1 + \dots + K_n + p_1^{(f)} + p_2^{(f)} - p_1^{(i)} - p_2^{(i)}) \times \\ \times \delta(p_{1\mu}^{(f)} p_{1\mu}^{(i)} - M^2) \delta(p_{2\mu}^{(f)} \dots) \delta(K_{1\mu} K_{1\mu}^* - m^2) \dots \delta(K_{n\mu} K_{n\mu}^* - m^2) f \quad (11)$$

where m is the mass of the mesons and where A takes into account the various conservation laws (such as isotopic spin, baryon number, strangeness) and the statistical factors due to the indistinguishability of the identical created particles.

The "statistical model" can be formulated by postulating that f is independent of the momenta and of the nature and multiplicities of the initial and final states of the particles. Therefore: f = const. If in Eq. (11) one calculates the integrals over the energy variables $d p_{1\mu}^{(f)} \dots d K_{n\mu}$, one obtains the explicit dependence of the transition probability on the phase-space factor:

$$\int \frac{d^3 p_1^{(f)}}{\sqrt{\vec{p}_1^{(f)2} + M^2}} \dots \frac{d^3 K_n}{\sqrt{K_n^2 + m^2}} S^2(\vec{K}_1 + \dots - \vec{p}_2^{(i)}) .$$

In the statistical model this factor determines the relative transition probabilities. But in order to obtain a physically meaningful theory, it is necessary to state, in addition, in which reference frame the separation of space and time is made. We shall assume that, for the statistical model, the calculation of the phase factors must be done in the CM system. The explicit formula which introduces in the S-matrix formalism the assumption that the phase-space factors must be calculated in the CM frame will be given later.

Now in order to calculate the relative transition probabilities in a multiple production process, maintaining fixed the initial and final nucleon momenta

$$\vec{p}_1^{(i)} \vec{p}_2^{(i)} \vec{p}_1^{(f)} \vec{p}_2^{(f)}$$

it suffices to evaluate in the CM system the following invariant phase-space factor. For the sake of simplicity we shall assume

$$\vec{p}_1^{(f)} + \vec{p}_2^{(f)} = 0$$

and the inelasticity, $K \approx 1$.

One can use the following recurrence relation in the CM system.⁵
The invariant phase-space factor R_n is:

$$R_n(P) = \int \prod_{r=1}^n d^4 K_r \delta(K_r^\mu K_r^\nu - m^2) \delta^4(K_1 + \dots + K_n - P).$$

In the CMS:

$$R_n(O, E) = \frac{1}{2} \int \frac{d^3 K_n}{(K_n^2 + m^2)^{1/2}} R_{n-1}(O, E) \quad (12)$$

where:

$$\epsilon^2 = (E - \sqrt{K_n^2 + m^2})^2 - \vec{K}_n^2.$$

Noting that

$$\frac{d^3 K_n}{\sqrt{K_n^2 + m^2}}$$

is the differential phase-space factor corresponding to the n th particle, one obtains from Eq. (12) the spectral distribution in the CM system of the created mesons.

The calculations based on this formula give reasonably correct answers in cases of one pion production near the threshold, and in the case of a nucleon-anti-nucleon annihilation if one takes into account the isobaric state $(3/2, 3/2)$ of the nucleons. This means that in the low energy region the assumption $f = \text{const.}$ is approximately verified; and, from the nonlocal point of view, the relativistic cut-off factors can be put $= 1$ (since in the calculation no high values of momenta occur). For high energy jets, the statistical model is not in accord with experimental data. This follows immediately from the anisotropy observed in the CM system since statistical factors can explain only an isotropic distribution. The anisotropy must be due to the nature of the interaction, for example, to the dependence on the total angular momentum or on the special structure of the interaction Hamiltonian (or Lagrangian). Also the predicted multiplicity and average transverse momentum are not in accord with observations. Indeed, one obtains for high energy jet an asymptotic expression for the probability W_n of finding a multiplicity n of the type:

$$W_n = A \frac{\Omega^{n-1} (4n-4)! E^{3n-4}}{\pi^{2n-2} 2^{4n-4} (2n-1)!(2n-2)!(2n-3)!} \simeq A \frac{\Omega^{n-1/2} (2\pi^3)^{1/2}}{\pi^{2n} (n)(3n-4)!(4n-3)!} E^{3n-4} \quad (13)$$

where $E = (E_1^{(i)} + E_2^{(i)})$ is the total energy in the CM frame.⁶

The probability ω_n is maximum for low values of n . Since from experiments we know that the inelasticity coefficient K is ~ 0.5 , one obtains from the above value n high average values of the energies K_{ν_0} ($\nu = 1 \dots n$) of the created mesons which is also in contrast with the experiments. If, for instance, $E = 100$ Bev, the probability of finding a pion of 20 Bev would be much greater than of finding a pion of 0.5 Bev, contrary to the experiment.

From the previous discussion, it is evident that the interaction between nucleons and mesons depends upon the total energy and upon the relative momenta of the interacting particles in the CM system. Thus, the interaction Hamiltonian or Lagrangian must not only be a function of the coordinate differences, but also of the momentum operators.

However, the most important deduction from the experimental data on the momentum distribution in the CM system is the following: let us consider jets, in which the total energy released in the CM frame is $\gtrsim 100$ Bev. One could expect that some created particle comes out with energy of this order of magnitude. But the experiment shows that the great majority of created particles have momenta (in CM system) of ~ 1 Bev or less. Pions of 10 Bev are rare exceptions. Thus, since the amount of the energy released is sufficient to produce many particles with energy ~ 10 Bev, there must be a reason why the probability of states of high momenta is much smaller than the probability of states of low momenta. Since this situation is encountered in many different types of interactions, one is inclined to attribute the cause not to the specific interaction Hamiltonian, but to the statistical weight of the states of the particles.

The basic assumption of the nonlocal theory, which will be discussed below, is that the statistical weight of a non-degenerated stationary eigenstate of the energy of particle is not always = 1 (in the CM system) but is given by a universal function, which defines the cut-off factors.

The following remarks can be added in order to support this assumption. The general expression (11) of the transition probability contains the S-matrix elements, $\langle |M| \rangle$, which for low values of the momenta give $f = \text{const.}$, independent of the final values of the momenta. This dependence is left to the phase-space factors. The disagreement between this simple statistical model and the observational data disappears if the phase-space factors are conveniently modified.

It is well known that the self-energy is infinite in a local field theory. On the other hand, if one introduces a momentum cut-off factor in the matrix element of the interactions as a weight-factor for the intermediate states, one can calculate the mass differences of some elementary particle pairs in accord with the experimental values as was shown by Feynman and Speiser in the case of a charged and a neutral pion and of the proton-neutron. Such calculations, based on a convenient choice of the cut-off function and of the universal length, show that the virtual

processes in which high momenta in the CM system are involved contribute with a reduced statistical weight to the value of self-energies or of mass differences, in agreement with the assumption of nonlocal field theory.

The suggested models and theories of multiple production of particles are due to Heisenberg,⁹ to Lewis, to L. Oppenheimer and Wouthuysen,¹⁰ to R. Glauber,¹¹ to E. Fermi,¹² to Landau,⁷ and to many other physicists.⁵ It is not the purpose of the present lectures to criticise these attempts. In my opinion, none of them has the character of a new field theory, which includes the present local theories at low energies yet correcting their unsatisfactory aspects (as the divergencies and the subtraction of infinite constants in renormalization processes). We shall not give an account of the historical development of these ideas.

IV. Basic Assumptions of a Nonlocal Theory of Field

In a local field theory one assumes that a particle can be "localized" at a point

$$x_\nu = (\vec{x}, t)$$

with arbitrary precision. Therefore an interaction of the type one encounters in electrodynamics between a current 4-vector

$$\bar{\Psi} \gamma_\mu \Psi$$

and a 4-vector potential A_μ can be represented by

$$e \bar{\Psi}(x) \gamma_\mu \Psi(x) A^\mu(x) = \\ = e \int d^4x' d^4x'' d^4x''' A^\mu(x) \delta^4(x'-x) \bar{\Psi}(x') \delta^4(x''-x) \gamma_\mu \Psi(x'') \delta^4(x'''-x) \quad (14)$$

where the Dirac functions $\delta^4(x'-x)$ etc. characterize the local interactions at the point x . The obvious generalization consists in the replacement of

$$\delta^4(x'-x) \delta^4(x''-x) \delta^4(x'''-x)$$

by some more general invariant function

$$F(x'-x, x''-x, x'''-x)$$

called a form-factor, (e. g., F could be a Gaussian function of the invariants $(x'-x)^2$, etc.).

The formalism of a nonlocal field theory containing some form factor requires the revision of the whole S-matrix and the Hamiltonian formalism. Starting from the idea that instead of point interaction in space time one can produce interactions defined in 4-dimensional domains

D_l (depending in their extension on a new universal constant

$$\ell = M^{-1} \sim 2 \cdot 10^{-14} \text{ cm.}),$$

one is led to the conclusion that inside such domains the possibilities of space and time measurements are limited in a new way. For example, we could not observe the propagation of free fields inside a domain D_l and therefore must limit ourselves to an approximate description of the propagation in domains substantially greater than D_l . The situation is similar to the problem of representation of the evolution with time of a quantum states of a particles by means of a succession of uncertainty domains, or "cells"

$$(\Delta p \Delta q)^3 \sim h^3$$

in phase-space, each corresponding to one state.

No such limitation arises if we use the representation of states in the p -space. Thus in the study of the interaction between particles and of such phenomena as scattering or "self-energy" problems, we shall be able to apply a stationary Schrödinger equation in the momentum variable p , and the S-matrix formalism.

What are the main difficulties in establishing a consistent, nonlocal, relativistic, field theory? Some of them arise from the claim of macroscopic causality, others from the quantum theory of measurement in space and time associated with the known properties of the Lorentz transformation in space and time.

Let us begin with two remarks concerning the second kind of difficulties. The measurement of a spatial distance with an error

$$\Delta x < \ell$$

requires the use of wavelengths:

$$\lambda = 2\pi \ell = 2\pi p^{-1} < \ell ; (l_p > 2\pi).$$

The Abbe formula,

$$\Delta x \gtrsim \frac{\lambda}{\sin \alpha} ,$$

is compatible with Δx arbitrarily small. But if the measuring devices are such that for

$$l_p > 2\pi$$

α is bounded by

$$\alpha \lesssim 2\pi(l_p)^{-1},$$

then

$$\Delta x \gtrsim \frac{2\pi p^{-1}}{2\pi(l_p)^{-1}} = l.$$

Now an analysis of high energy interactions of the type observed in jets reveals that the above condition is verified for the secondary particles of a jet.¹⁵ If, for example, one thinks of an n-n collision in which high energy nucleons are used in order to localize the position of a proton, if one studies the structure of this proton in the sense of a Heisenberg microscope experiment, then the error, Δx , is determined by the wavelength, λ , of the secondary particles of the jet and by the smallness of the angles α formed by these particles. As we have seen, $\lambda \sim l$ in CM system, and

$$\alpha \lesssim \frac{p_{\perp}}{p_{\parallel}} \sim \frac{l}{l_p}$$

if high values

$$l_p \gg 1$$

are used. Thus,

$$\Delta x \gtrsim l.$$

Similar considerations are valid if one considers the average value of the scattering angle ϑ in elastic scattering processes, such as Compton or Moeller scattering. Therefore, there is no contradiction between the Heisenberg's uncertainty relations and the assumption of the existence of a universal lower limit of measurable length.¹³

The second remark concerns the Lorentz contraction. Any length appears in some suitable reference frame contracted by a factor which can be arbitrarily chosen

$$(\gamma = (1 - \beta^2)^{-\frac{1}{2}}).$$

If, for instance, we want to define a "short range" interaction, it will be necessary to take into account the full dynamical description of the interacting particles because the assignment of their simultaneous position is insufficient. Indeed let us suppose that one observer finds the distance between two neutrons at rest

$$|\bar{x}' - \bar{x}''| = (1 \pm \Delta x) \text{ cm}$$

(their momenta satisfying the uncertainty relations). There are other observers who will find the corresponding distance contracted to values, e. g., less than 10^{-13} cm and their velocities changed correspondingly. The question of whether and when these observers will find the two particles interacting depends not only on their positions but also on the relative velocities. By choosing the initial neutron momenta conveniently, one easily can analyze different possible cases. The important conclusion concerning the introduction of elementary interaction domains, D_7 , is that the full dynamical description of interacting particles is necessary in such cases, and the unambiguous distinction between small distances and large distances will be conveniently defined in the CM system of the interacting physical particles.

The basic assumptions of the nonlocal field theory can be formulated in a simple way if, in accord with Bohr's complementary principle and Heisenberg's uncertainty relations, we separate the approximate description of the propagation in macroscopic space-time domains of "physical particles" from the description of short range interactions in which an exchange of momenta, angular momenta or charges takes place, or, more generally, in which particles are created and destroyed. The definition of the physical particles will be found below. In this initial discussion we shall avoid the consideration of long range fields and shall examine strong short range interactions of the type encountered between nucleons and mesons.

Starting with the hypothesis of the existence of universal interaction domains, D_7 , which are also domains of uncertainty for space and time measurements, and with the idea that particles are not localizable but have extensions and structures, we are led naturally to the conclusion that the description of propagation of a particle in space-time must have a limited precision. Indeed, according to quantum theory it will be sufficient to describe approximately the propagation of wave-packets of probability amplitudes in a way adequate to represent interference and diffraction phenomena and some effect of "external" classical fields. This sufficiency is connected with the quantum and atomic structure of reference systems and measuring devices.¹⁴

Thus, the free field equations of propagation must represent the motion of one "physical" particle not interacting strongly with other physical particles, and thus containing "renormalized" charges and masses obtained from measurements in the low energy region.

If one assumes the existence of 4-dimensional domains of interaction where the creation and destruction of particles takes place, it seems obvious that in such domains one can neither apply the propagation equations nor have macroscopic causality. We shall associate the assumption that these domains have in the CM system of incoming interacting particles an extension of $\sim l^4$ with the assumption that there are

no fundamental particles having a mass substantially greater than the nucleon mass M , and thus shall put

$$\mathcal{I} = M^{-1} \cong 2 \cdot 10^{-14} \text{ cm.}$$

On the other hand the description of interaction can be given in the momentum space. We shall adopt a Hamiltonian formalism assigning a Hamiltonian operator H_0 for each free field as a function of momenta p_μ , and of spin and other internal parameters, and an interaction Hamiltonian H' which can also be expressed as a function of momenta p_μ , and of spin and other internal parameters.

Two types of problems will be solved by the use of the S-matrix formalism in p -space: the self-energy problem and the scattering processes.

Let us consider a collision between particles having known momenta, spin, polarizations, etc., and represent them as plane wave solutions of the free particle equations. Let

$$P_\mu = \sum_i p_\mu^{(i)}$$

be the total energy-momentum 4-vector (see Section I) and let u_μ be the velocity-vector of the center of momenta (CM) system of the ingoing colliding particles:

$$u_\mu = \frac{1}{m} P_\mu, \text{ where } m^2 = P_\mu P^\mu > 0. \quad (15)$$

We shall introduce the following invariant projections of any 4-vector k_ν :

$$I_t(k) = k_\nu u^\nu \quad I_s = \sqrt{I_t^2 - k_\nu k^\nu} \quad (16)$$

and shall call them respectively the projection on the time-axis (or energy axis) of the CM system and "projection" on the space of the center of momenta system, because in the CM system one has:

$$u_\nu = (1, 0, 0, 0)$$

$$I_t(k) = k_0$$

$$I_s(k) = \sqrt{k_1^2 + k_2^2 + k_3^2} = |\vec{k}|. \quad (16')$$

Introducing operators-functions of these invariants in the interaction Hamiltonian, one can modify in a covariant way the usual S-matrix formalism. A convenient choice of these relativistic cut-off operators

in the p -space is equivalent to the definition of the interaction domains D_1 in the space-time.

Referring to the example of a nucleon interacting with the pion field, we shall use following representation of a "physical" nucleon, surrounded by a pion cloud:

$$|n\rangle = (Z_n \Psi_n^*(\vec{p}) + \sum c_i(\vec{p}_i, \vec{k}_i) \Psi_n^*(\vec{p}_i) \varphi^*(\vec{k}_i) + \\ + \sum c_2(\vec{p}_2, \vec{k}'_2, \vec{k}''_2) \Psi_n^*(\vec{p}_2) \varphi^*(\vec{k}'_2) \varphi^*(\vec{k}''_2) + \dots) |O\rangle . \quad (17)$$

Here

$$\Psi_n^*(\vec{p})$$

and

$$\varphi^*(\vec{k})$$

are creation operators of a free nucleon and a pion in states characterized by the momenta \vec{p} and \vec{k} , and $|O\rangle$ represents the vacuum of "bare" particles (eigenstates of the free Hamiltonian with non-renormalized masses and charges). In a similar way the physical state of a pion can be represented as follows:

$$|\pi\rangle = (Z_\pi \varphi^*(\vec{k}) + \sum a_i(\vec{p}'_i, \vec{p}''_i) \Psi^*(\vec{p}'_i) \Psi^*(\vec{p}''_i) + \dots) |O\rangle . \quad (18)$$

In the above formulae

$$Z_n, c_i, Z_\pi, a_i, \dots \text{etc.}$$

are the probability amplitudes for finding a bare nucleon, or a nucleon with one meson, or a bare meson, or a nucleon anti-nucleon pair respectively.

In the following we shall illustrate the method of relativistic cut-off (or of nonlocal fields) by studying a very simple case, the "Lee model," for which we shall be able to write the stationary Schrödinger equation and solve it exactly.

V. The Relativistic Lee Model

Let us consider 3-scalar fields of V , N , φ particles and assume that the interaction Hamiltonian describes the elementary processes,

$$V = N + \varphi$$

Following Lee, let us examine separately the "sectors" satisfying the conditions:

$$n_V + n_N = C_1 = \text{const.} \quad n_N - n_{N^*} = C_2 = \text{const.} \quad \text{and put: } C_1 = 1; C_2 = 0.$$

Introducing from the beginning the cut-off operators, we can solve the stationary Schroedinger equation in p-space:

$$\begin{aligned} H &= H_0 + H' \\ H|V\rangle &= (H_0 + H')|V\rangle = E|V\rangle \quad (19) \\ H_0 &= \sum_{\vec{p}} E_V(\vec{p}) \psi_V^*(\vec{p}) \psi_V(\vec{p}) + \\ &\quad + \sum_{\vec{k}'} E_N(\vec{k}') \psi_N^*(\vec{k}') \psi_N(\vec{k}') + \sum_{\vec{k}} \omega(\vec{k}) a^*(\vec{k}) a(\vec{k}). \end{aligned}$$

Here H' is the interaction Hamiltonian in which relativistic cut-off operators are introduced as functions of the invariants I_t , I_s and $|V\rangle$ is the eigenstate of the system defined as a superposition of eigenstate of the free Hamiltonian H_0 containing non-renormalized masses. Indicating by Ω the 3-dimensional volume, to which the second quantization of free fields is referred and by g_0 the non-renormalized coupling constant we can write:

$$\begin{aligned} H' &= -\frac{g_0}{\sqrt{\Omega}} \sum_{\vec{k}+\vec{k}'=\vec{p}} \frac{1}{\sqrt{2\omega(\vec{k})}\sqrt{2E_N(\vec{k}')}\sqrt{2E_V(\vec{p})}} \cdot \\ &\quad \cdot \left\{ f \psi_V^*(\vec{p}) \psi_N(\vec{k}') a(\vec{k}) + f^* \psi_V(\vec{p}) \psi_N^*(\vec{k}') a^*(\vec{k}) \right\} \quad (19') \end{aligned}$$

where the operators

$$a(\vec{k}), \psi_N(\vec{k}'), \psi_V(\vec{p})$$

satisfy the commutation relation:

$$\begin{aligned} [a(\vec{k}), a^*(\vec{k}')] &= \delta(\vec{k}, \vec{k}') \quad \text{etc.} \\ [a(\vec{k}), \psi_V(\vec{p})] &= 0 \quad \text{etc.,} \quad (20) \end{aligned}$$

and the cut-off operators f and f^* are defined as follows: to each creation-- or destruction--operator is associated a "spatial" cut-off factor:

$$G_s(I_s(\vec{k})) = [1 + I_s^2(\vec{k})]^{-1} = \left(\frac{1}{1 + (\vec{k})^2} \right)_{CM}. \quad (21)$$

To each vertex point (one of the terms of Eq. (19')) is associated a "time-form-factor":

$$G_t = g^-(I_t(lk) + I_t(lk'))g^+(I_t(lp)); \quad \text{or} \quad (22)$$

$$G_t^* = g^-(I_t(lp))g^+(I_t(lk) + I_t(lk'))$$

where:

$$g^- = \frac{1-i(\sum M)}{1+i(\sum I_t)} \quad g^+ = \frac{1+i(\sum M)}{1+i(\sum I_t)} \quad (22')$$

are associated with destruction or with creation operators respectively. Hence the operators f and f^* are:

$$f = G_s(p)G_s(k')G_s(k)G_t \quad f^* = G_s(p)G_s(k)G_s(k)G_t^*. \quad (23)$$

In more general cases the interaction Hamiltonian H' will contain other terms of the type:

$$\Psi_v^* \Psi_N^* a_k^*$$

or

$$\Psi_v \Psi_N^* a_k \quad \text{etc.}$$

But we shall limit our relativistic Lee model to represent three boson scalar fields for which only the reactions



are possible. We exclude also the negative energy states.

Let us solve the self-energy problem of the V particle. We assume that the physical state $|V\rangle$ of the V particle can be represented as a superposition of bare states of V , N , ν :

$$|V\rangle = N \left(\Psi_v^*(0) + \frac{q_0}{i\Omega} \sum_{\vec{k}} \Phi(\vec{k}) \Psi_N^*(-\vec{k}) a^*(\vec{k}) \right) |0\rangle. \quad (24)$$

Here we already have introduced the CM system of the V particle ($\vec{p}=0$) and have taken into account the momentum conservation by putting $\vec{k}'=-\vec{k}$. $\Phi(\vec{k})$ defines the cloud of N and ν particles around V , and N is the normalization constant which defines the renormalized coupling

constant, $g = g_0 N$.

Our problem is reduced now to the solution of the following stationary Schroedinger equation:

$$(H_0 + H')|\psi\rangle = E|\psi\rangle. \quad (19'')$$

Substituting Eq. (24) into Eq. (19''), one obtains by an elementary calculation the following two equations:

$$(M_v - E) - \frac{g_0^2}{\Omega} \sum_{\vec{k}} \frac{f \cdot \phi(\vec{k})}{\sqrt{2M_v} \sqrt{2E_N} \sqrt{2\omega_k}} = 0 \quad (25)$$

$$(E_N(-\vec{k}) + \omega(\vec{k}) - E) \phi(\vec{k}) = \frac{f^*}{\sqrt{2M_v} \sqrt{2E_N} \sqrt{2\omega_k}}$$

and assuming

$$M_N + M_{v^2} > M_v > E,$$

one obtains the eigenvalue E from

$$(M_v - E) = \frac{g_0^2}{\Omega} \sum_{\vec{k}} \frac{ff^*}{8M_v E_N \omega_k} \frac{1}{(E_N + \omega_k - E)}. \quad (25')$$

Then the spectral distribution function

$$\phi(\vec{k})\phi^*(\vec{k})$$

can be computed from Eq. (25).

The normalization condition

$$\langle \psi | \psi \rangle = 1$$

gives:

$$N^2 \left[1 + \frac{g_0}{\Omega} \sum_{\vec{k}} \phi(\vec{k})\phi^*(\vec{k}) \right] = 1 \quad (26)$$

or

$$N^2 = 1 - \frac{g^2}{\Omega} \sum_k \frac{ff^*}{8M_V E_N \omega_k} \frac{1}{(E_N + \omega_k - E)^2}. \quad (26')$$

Introducing the following values for the constants

$$\lambda = 1 \quad M_N = 1 \quad M_{\omega} = 1, \quad (27)$$

and thus

$$E_N = \omega_k = \sqrt{1 + k^2},$$

we obtain the cut-off operators,

$$\begin{aligned} f &= G_s^2 G_t = \frac{1}{(1+k^2)^2} \frac{1-2i}{1-i2\sqrt{1+k^2}} \\ f^* &= G_s^2 G_t^* = \frac{1}{(1+k^2)^2} \frac{1+2i}{1+i2\sqrt{1+k^2}} \\ ff^* &= \frac{1}{(1+k^2)^4} \frac{1}{(1+\frac{4}{5}k^2)} ; \quad \lim_{k \rightarrow 0} f = \lim_{k \rightarrow 0} f^* = 1 \end{aligned} \quad (28)$$

and by passing to the limit of continuum,

$$\frac{1}{\Omega} \sum_k \longrightarrow \frac{1}{(2\pi)^3} \int d^3 k, \quad ,$$

we get finally:

$$M_V(M_V - E) = \left(\frac{g_0}{4\pi}\right)^2 I_1(E)$$

$$N^{-2} = 1 + \left(\frac{g_0}{4\pi}\right)^2 I_2(E)$$

where

$$I_1(E) = \int_0^\infty \frac{k^2 dk}{(1+k^2)^5 \left(1 + \frac{4}{5}k^2\right) [2\sqrt{1+k^2} - E]} \quad (29)$$

$$I_2(E) = \int_0^\infty \frac{k^2 dk}{(1+k^2)^5 (1+\frac{4}{3}k^2)[2\sqrt{1+k^2}-E]^2} = \frac{dI_1}{dE} .$$

The problem of scattering of one ν^2 particle on one N particle can be solved in a similar way. The general state of the system

$$|N+\nu\rangle = \left(C_V \psi_V^*(0) + \frac{g_o}{\sqrt{\pi}} \sum_{\vec{k}} \phi(\vec{k}) \psi_N^*(\vec{k}) \alpha^*(\vec{k}) \right) |0\rangle \quad (30)$$

can be considered as a superposition of the states of a bare V particle and of pairs of N and ν^2 particles. By substituting Eq. (30) into Eq. (19''), one finds two equations which now must be solved, taking into account that the scattered waves are only outgoing waves and using the Dirac operator:

$$\left[P \frac{1}{\omega' - \omega} - i \pi \delta(\omega' - \omega) \right] .$$

From the inspection of the solution, one concludes that in the CM system the scattering is isotropic. For such an S-wave scattering one easily finds the phase-shift δ_o and the cross section σ :

$$t_g \delta_o = \frac{\frac{g_o^2}{4\pi} \frac{ff^*}{8M_V \omega_i^2} k_i}{\bar{h}(k_i)}$$

where

$$\bar{h}(k_i) = E_i - M_V + \frac{g_o^2}{(2\pi)^2 8M_V \omega_i^2} P \int \frac{ff^* k \omega d\omega}{\omega - \omega_i} \quad (31)$$

k_i and $(-\vec{k}_i)$ are the incident momenta

$$k_i = |\vec{k}_i| ; \quad E_i = 2\omega_i = 2\sqrt{1+k_i^2}$$

$$\sigma = 4\pi \frac{\left(\frac{g_o^2}{4\pi} \frac{ff^*}{8M_V \omega_i^2} \right)^2}{\left[\bar{h}(k_i)^2 + \left(\frac{g_o^2}{4\pi} \frac{ff^*}{8M_V \omega_i^2} \right)^2 \frac{1}{k_i^2} \right]} \quad (31')$$

Asymptotically in the high energy limit ($\omega_i \rightarrow \infty$) this elastic scattering cross section σ vanishes as $\sim \omega_i^{-26}$ as one can see from Eq. (26'). In the low energy limit $k_i \rightarrow 0$ one can expect from the definition of

domains D_l that

$$\sigma \rightarrow \pi l^2 = \pi.$$

In this case, if $M_y=1$, then

$$\frac{g_0^2}{4\pi} = 4.$$

Hence the choice of parameters of the problem is limited. One finds easily the following conditions:

$$\begin{aligned} M_v(2-M_v) &\cong \frac{g_0^2}{4\pi} \cdot \frac{1}{4} \\ M_v(M_v-E) &= \frac{g_0^2}{4\pi} \cdot \frac{1}{4\pi} I_1(E). \end{aligned} \tag{32}$$

One possible set of values is:

$$M_v=1; \quad \frac{g_0^2}{4\pi} = 4; \quad (g_0 \sim 7); \quad E = 0.990; \quad N^2 = 0.998.$$

VI. Form Factors and Causality

Obviously the above method can be generalized to arbitrary fields and to other types of interaction. But difficulties arise when we do not know how to solve the Schrödinger stationary equation and begin to use the perturbation method or some other approximation. I shall not discuss these difficulties because no satisfactory solution of them is known. In the few cases we shall consider, the assumption will be made that the few lowest terms of the perturbation solution gives a satisfactory answer, as it happens in electrodynamics.

The choice of the form factor, e. g., adopted in the example of the Lee model, is very important for a consistent nonlocal theory. Let us see how this choice can be justified. The value of the universal length

$$l = M^{-1} = 2 \cdot 10^{-14} \text{ cm}$$

is suggested by the calculation of pion-mass difference and proton-neutron mass difference, as well as by the theoretical interpretation of Hoffstadter's experiments on the charge and magnetic momentum distribution in nucleons and, also, by the mesonic theory of nuclear forces. The particular choice, Eq. (21), of the form factor is suggested by the theoretical interpretation of the Hoffstadter experiment. The angular distribution for electrons having the energy E in L system can be written:¹⁵

$$\frac{d\sigma}{d\Omega} = \frac{\alpha^2}{4E^2} \frac{\cos^2 \frac{\varphi}{2}}{\sin^2 \frac{\varphi}{2}} \frac{1}{\left(1 + 2 \frac{E}{M} \sin^2 \frac{\varphi}{2}\right)} \left\{ F_1^2(q^2) + \frac{q^2}{4M^2} \left(2[F_1 + \mu F_2]^2 t q^2 \frac{\varphi}{2} + K^2 F_2^2 \right) \right\}$$

where

$$q^2 = -q_\mu q^\mu = \frac{(2E \sin \frac{\varphi}{2})^2}{\left(1 + 2 \frac{E}{M} \sin^2 \frac{\varphi}{2}\right)}$$

is the momentum transferred and μ is the anomalous moment of the proton or neutron. The form factors $F_1(q^2)$ and $F_2(q^2)$ are of the exponential type and their Fourier transform corresponds to our G_S cut-off factor. This explains the choice of the statistical weight factor in the CM system as

$$G_S = (1 + I_S(lk))^{-1}$$

The choice of the "time--" cut-off operators G_t , G_t^* is made in a way to satisfy the claim of macroscopic causality and the requirement that no signal can travel with velocity greater than c . The discussion of this point can be found in the literature.¹⁶ I want to stress that the cut-off operators G_t , G_t^* act in a different way on the created and on the absorbed particles. They do not mix outgoing and ingoing waves, and one obtains, starting from a point of the interaction domain D_I only outgoing waves for future times, and arriving at points of D_I only ingoing waves from the past. Therefore, no contradiction with the macroscopic causality can arise. But obviously in such approximate theory one cannot verify the microscopic causality inside the domains D_I . Note that the Fourier transform of a $g^+ = (1 + l \sum I_t(lk))$, in the CM frame, is a function of the proper time t of the CM system, which for $t < 0$ is 0, and for $t > 0$ is

$$\frac{1}{l} e^{-t/l},$$

whereas

$$g^- = (1 - i \sum I_t(lk))$$

has a Fourier transform, which is 0, for $t > 0$, and is

$$\frac{1}{l} e^{t/l}$$

for $t < 0$.

The Hamiltonian H^{19} modified by the introduction of the above form-factors remains Hermitian because the cut-off operators f and f^* are complex conjugate operators. The S-matrix remains also unitary.¹⁶

In electrodynamics the gauge-invariance for equations representing the propagation in space and time of noninteracting physical particles is obviously preserved. The G_s 's operators can be interpreted as weight factors in the statistics of a stationary system.

One can illustrate the significance of the relativistic cut-off factors in high-energy events for the Compton effect calculated to the lowest (2nd order) of the perturbation theory (neglecting radiative corrections and double Compton scattering and all higher order processes). Then we have to calculate the elastic scattering of a photon and an electron in the CM system, taking into account the 2nd order processes indicated in Fig. 7a, b. If

$$K_\nu \ P_\nu , K'_\nu \ P'_\nu$$

are the 4-momenta of the incident and the scattered particles respectively, one has: $\vec{P} + \vec{K} = 0 = \vec{P}' + \vec{K}'$; $|P| = |P'| = K_0 = K'_0 = \omega$.

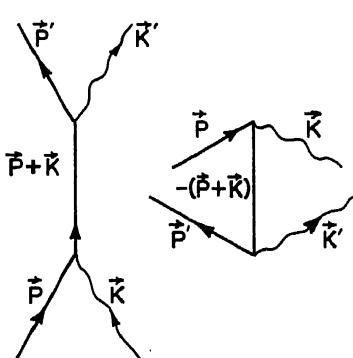


Fig. 7 a

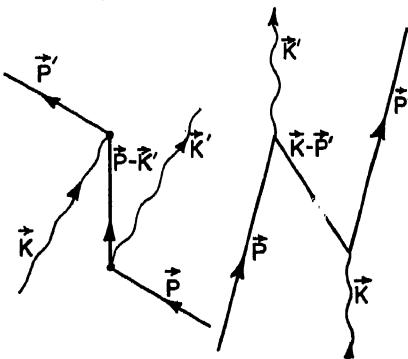


Fig. 7 b

In the well-known S-matrix element corresponding to Fig. 7 a, one inserts a common cut-off factor:

$$G_S^4(l(\vec{R})) g^- g^+ [\bar{l}(P_0 + K_0)] = \frac{1}{(1 + l^2 \omega^2)^4} \frac{1 + l^2 m_e^2}{1 + l^2 (P_0 + \omega)^2} \quad (33)$$

$$[G_S^2(l(\vec{P} + \vec{K})) = 1 \text{ etc.}] .$$

The element corresponding to the second pair, Fig. 7b, receives a different cut-off factor:

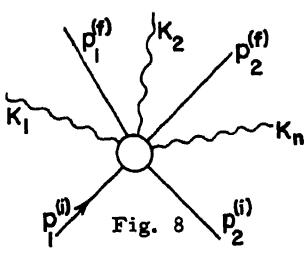
$$G_s^4 (\ell | \vec{K} |) G_s^2 (\ell (\vec{P} - \vec{K}') g^- g^+ (\ell P_2) g^- g^+ [\ell (\vec{P} - \vec{K}') + \omega]) \quad (33')$$

If one takes into account the known expression of the S-matrix elements corresponding to all these diagrams, one finds that in the limit $\omega \gg \ell$ the Compton cross section vanishes much more rapidly than in the case of Klein-Nishima-Tamm formula and that the term corresponding to the first two diagrams becomes dominant for

$$K_s = \omega \gg \ell^{-1}$$

in the CM system, and gives a contribution to $d\sigma/d\Omega$, which tends to 0 as $\omega^{-1/4}$. Only for a scattering angle $\theta = \pi$ do the other Feynman diagrams give contributions to $d\sigma/d\Omega$ of order of magnitude as the first.

VII. A Theory of Multiple Production



If

$$|\langle K_1 \dots K_n | P_1^f P_2^f | M | P_1^i P_2^i \rangle|^2 = |M|^2$$

is the square of the element of the transition matrix in p-space, it will contain one statistical weight factor

$$G_s^2 (I_s (\ell K))$$

for each external line, and also the following "time cut-off" operators:

$$g^- (I_t (\ell P_1^i) + I_t (\ell P_2^i)) = (g^- [\ell (E_1^i + E_2^i)])_{CM} \quad (34)$$

$$g^+ \left(\sum_{r=1}^n I_t (\ell K_r) + I_t (\ell P_1^f) + I_t (\ell P_2^f) \right) = (g^+ [\ell (\epsilon_1 + \dots + \epsilon_n + E_1^f + E_2^f)])_{CM}$$

From the above definitions of the cut-off operators we can establish the following cut-off rules in the case of a general diagram, Fig. 8, in which $n+2$ external outgoing lines represent the n created particles and the two final states of nucleons whereas 2 ingoing external lines represent the incident nucleons.

Together the g^- and g^+ give a real cut-off factor:

$$\left(\frac{1 + l^2(\sum M)^2}{1 + l^2(\sum E)^2} \right)_{CM}. \quad (34')$$

All other cut-off operators will give rise to real cut-off factors in all propagators corresponding to internal lines of the diagram in the p -space. The properties of the modified propagators are described in Reference 16.

The $|M|^2$ must be summed over the subset of final states, which we wish to consider in the definition of the partial cross section, or over all final states, if we wish the total cross section. The internal coordinates (spin-components, charges, etc.) can be fixed for initial and for final states (or $|M|^2$ can be conveniently averaged and summed in the usual way).

If we sum up with respect to all final states of K_1, \dots, K_n

$$W_n = \int |M|^2 \delta^4(K_1 + \dots + K_n + p_1^f + p_2^f - p_1^i - p_2^i) d^3 K_1 \dots d^3 K_n \quad (35)$$

the G_s, G_t cut-off factors of external lines can appear explicitly in W_n :

$$W_n = \int |X|^2 \frac{\delta^4(K_1 + \dots + K_n + p_1^f + \dots - p_2^i)}{[1 + l^2(\sum I_t)^2]} G_s^2(lK_1) \frac{d^3 K_1}{\epsilon_1} \dots G_s^2(lK_n) \frac{d^3 K_n}{\epsilon_n} \quad (36)$$

where we have also put in evidence the factors

$$\epsilon_r = \sqrt{K_r^2 + m_r^2}$$

which came from the representation of final states in the p -space. The 4-dimensional expression of Eq. (36) is:

$$W_n = \int |X|^2 \frac{\delta^4(K_1 + \dots + K_n + \dots - p_2^i)}{[1 + l^2(\sum I_t)^2]} G_s^2(I_s(lK_i)) \cdot \\ \cdot d^4 K_1 \delta(K_1^2 - m_1^2) \dots d^4 K_n \delta(K_n^2 - m_n^2). \quad (36')$$

If we put in Eq. (36) $|X|^2 = \text{const.}$, we obtain the formalism of a "statistical theory with cut-off" possessing following properties: the mesons spectrum in the high energy jets is given approximately by

$$\frac{dn}{d|K|} \sim \frac{l^2 K^2}{\sqrt{K^2 + m^2} (1 + l^2 K^2)^2} \quad (37)$$

which is approximately in accord with the observed spectrum of mesons in jets.

If, from the particular cut-off factors Eqs. (21) and (22'), one estimates the average dimensions, e. g., of the charge distribution in the case of a proton, one finds that the corresponding form factor in the configuration space gives

$$\sqrt{\langle r^2 \rangle} \sim 8 \cdot 10^{-14} \text{ cm.} \sim 4 l$$

in accord with the experimental value of Hoffstadter. If $|x|^2 = \text{const.}$, the angular distribution of the produced mesons in the CM system appears isotropic and the average multiplicity is in accord with the observations in the low energy domain:

$$(E_1^{(i)} + E_2^{(i)})_{\text{CM}} < 10M .$$

In this region, if the final momenta $|\vec{k}_1| \dots |\vec{k}_n|$ are $\lesssim M$, the cut-off factors G_S^2 are ~ 1 , and the statistical model can give reasonable results.

But the experiments (see Section II) show that in the high energy region, where

$$(E_1^{(i)} + E_2^{(i)})_{\text{CM}} \gtrsim 10^3 M ,$$

the angular and momentum distribution of produced particles is anisotropic. Such behaviour can be ascribed only to the interaction Hamiltonian H' or to the structure of the elements

$$\langle K, \dots K_n | p_1^f p_2^f | M | p_1^i p_2^i \rangle$$

of the S-matrix.

One plausible theory of these multiple production events can be based on the assumption of the existence of a nonlinear Hamiltonian, which in the low energy region is reduced approximately to the usual linear coupling terms. Such Hamiltonians were considered in connection with the theory of multiple production by R. Glauber.¹¹

The main point in our treatment is that these nonlinear Hamiltonians are necessary only in the description of high energy interactions in D_1 domains, and do not give rise to any modification of propagation equations of free fields (these last equations represent approximately the law of propagation of free fields outside the interaction domains, and we need not control their validity inside D_1).

We need to consider these nonlinear Hamiltonian operators exclu-

sively in the p-space in calculating the matrix elements of the S-matrix. The choice of such a nonlinear interaction cannot be fixed until a more consistent general theory of interaction is discovered and more knowledge is gained about the high energy events. But it is possible to show that these interactions can give rise to the multiple production in the high-energy collisions and that by a suitable choice of H' the resulting angular distribution is anisotropic. According to the well-known ideas suggested by Heisenberg,¹⁷ one can hope to obtain from a nonlinear spinor theory the masses and the coupling constants of all fields. Such a theory would very probably also lead to a correct interpretation of jets.

We start with the remark that in a nonlocal theory of the type sketched above the perturbation expansion can be reduced to few terms of lower order because the intermediate virtual states are cut off by the "time-cut-off" operators G_t and, being unstable, have a finite lifetime. The whole process represented by a given Feynman diagram of n-th order also has a lifetime $\sim l$ or less corresponding to a D_l domain having an extension $\sim l^4$ in CM system (a well-known Lorentz-contraction effect of the clouds of mesons around each of the colliding nucleons, reduces the total time interval of interaction). In ultra high energy collisions, probably only the first term of the perturbation expansion must be considered.

Therefore, the nonlinear Hamiltonian must have terms of the type:

$$H' = \sum f \cdot C_{K_1 \dots K_n} p_1^{\mu} p_1^{\nu} p_1^{\rho} \dots p_1^{\sigma} \frac{b(p_1^{\mu}) b^*(p_1^{\nu}) b(p_1^{\rho}) b^*(p_1^{\sigma}) \dots a^*(K_1) \dots a^*(K_n)}{\sqrt{2} p_1^{\mu} \dots \sqrt{2} \epsilon_n} \quad (38)$$

+ herm. conj.

In order to obtain the anisotropic angular distribution, we can build Hamiltonian (or Lagrangian) functions of the following new invariant

$$I_a = K_\mu v^\mu \quad (39)$$

where the 4-vector v_μ is

$$v_\mu = \frac{p_{1\mu}^{(i)} - p_{2\mu}^{(i)}}{\sqrt{(p_{1\mu}^{(i)} - p_{2\mu}^{(i)})^2 + (p_1^{(i)\mu} - p_2^{(i)\mu})^2}} \quad (39')$$

If the p_1 axis is parallel to the velocity of the initial nucleon and if the two incident particles have identical masses, then the components of v_μ in the CM system are: (0, 1, 0, 0) and the invariant I_a is the projection of the 4-vector K_μ on the axis of the jet. Now if the coefficients $C_{K_1 \dots K_n}$ contain an invariant factor

$$\prod_{r=1}^n I_a^{(r)} = (K_{\mu}^{(1)} v^{\mu}) \cdots (K_{\nu}^{(n)} v^{\nu})$$

(or some more complicated function of $I_a^{(r)}$)¹⁸ then the square of the matrix element derived from the Hamiltonian Eq. (38) will contain factors

$$\prod_{r=1}^n \cos^2 \vartheta_r$$

and the spectral distribution of one created meson will be given approximately by

$$\sim \frac{G^2(1|\vec{K}|)|\vec{K}|^4}{\sqrt{K^2 + m^2}} \cos^2 \vartheta d|\vec{K}| d(\cos \vartheta). \quad (40)$$

This distribution has the same anisotropy as that encountered in the "Turin jet."⁴ Obviously with another choice of the Hamiltonian, more general types of angular distributions (e. g., $\sim \cos^{2m} \vartheta$) can be obtained.

The nonlinear Lagrangians were introduced independently by many authors; a historical review of these nonlinear theories will not be attempted here, although some of the most significant contributions are listed in Reference 19. The main new point in the above solution of the multiple production problem is the separation of the space-time description from the formalism of the S-matrix in p-space, which makes possible the solution of the scattering and the self-energy problems within the frame work of a nonlocal theory. More detailed discussion of the possibilities offered by the nonlinear interaction Hamiltonians in p-space is outside the scope of these lectures.

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SELECTED TOPICS IN NUCLEAR THEORY

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I. The Many-Body Problem: The Relation of the Shell Model to the Basic Two-Body Forces

Historically, the first attempts to describe nuclei were based on the idea of a shell model, mainly because this description had been very successful in the case of the atom. However, the validity of such an approach seemed doubtful in view of the strength and the short range of the nuclear forces, as compared to the weaker long-range forces in the atom. These doubts were reinforced by the discovery of slow-neutron resonances, which clearly indicated the importance of many-body features which are neglected in the shell-model approach, and by the success of the compound-nucleus model of Niels Bohr, which in its extreme form idealizes the nucleus by treating it as a system of strongly interacting, and strongly correlated particles, like the molecules in a liquid drop.

Thus there was a period when most physicists were convinced that any shell model could, by purely theoretical arguments, be proved invalid. We shall examine these arguments in detail later on.

However, attempts to relate nuclear properties to a shell structure continued in spite of these objections. In particular, Maria Mayer was able to show the existence of regularities which clearly indicated the existence of closed shells ("magic numbers" of neutrons or protons) in nuclei; and finally she and, independently, Jensen and collaborators showed that the inclusion of a spin-orbit coupling in the field acting on each particle could account quantitatively for the values of the magic numbers, for the spin values of nuclei, and a number of other features.

This agreement was so impressive that it left no doubt that the shell model contained a good deal of truth. It remained therefore, firstly to reconcile this result with the theoretical objections, and secondly to determine from first principles how to carry out shell model calculations. This requires determining the potential well (including the spin-orbit part) which defines the shell states, and also the residual two-body forces which give rise to the corrections to the simple shell approximation and which are responsible for splitting the levels that in the first approximation are degenerate.

The understanding of these problems has advanced rapidly in the last few years, and the first section of this lecture course will be con-

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cerned with these topics.

The most obvious way of approximating to a many-body problem in terms of individual-particle wave functions is through the Hartree, or Hartree-Fock approximation, which works very satisfactorily for atoms. We shall see that this requires modification in the nuclear case, but it will nevertheless be useful to start by discussing the nuclear problem in terms of this method.

The simplest presentation of these methods starts from the variation principle, by which the energy of the ground state is given as the lowest value of the quantity

$$\bar{E} = \langle \Psi^* H \Psi \rangle / \langle \Psi^* \Psi \rangle \quad (1)$$

in which H is the complete Hamiltonian of the many-body problem and the brackets indicate integration over all coordinates. The ground-state wave function is the function which minimizes Eq. (1).

In the Hartree approximation we restrict ourselves to wave functions which are products of one-particle functions:

$$\Psi = u_1(\underline{x}_1)u_2(\underline{x}_2)\dots u_N(\underline{x}_N) \quad (2)$$

and look for that particular product function which gives the least value of Eq. (1). Substituting this into the variational equations we obtain a set of one-particle equations

$$\begin{aligned} -\frac{\hbar^2}{2m} \nabla^2 u_1 + [U_1(\underline{x}_1) - E_1] u_1 &= 0 \\ \dots \\ -\frac{\hbar^2}{2m} \nabla^2 u_N + [U_N(\underline{x}_N) - E_N] u_N &= 0 \end{aligned} \quad (3)$$

where the one-particle potentials U_j are defined in terms of the one-particle wave functions, so that we have to find the u_j and the U_j simultaneously, usually by trial and error:

$$\begin{aligned} U_j(\underline{x}_j) &= \sum_{i \neq j}^N \int V(\underline{x}_j - \underline{y}) |u_i(\underline{y})|^2 d^3y \\ &= U(\underline{x}_j) - \int V(\underline{x}_j, \underline{y}) |u_j(\underline{y})|^2 d^3y \end{aligned} \quad (4)$$

Care is needed in interpreting the one-particle energies E_j which occur in Eq. (3). The total energy Eq. (1) is not, as one might think,

equal to the sum of the one-particle energies, since in adding these the interaction potential is counted twice.

$$\sum_i E_i = \bar{E} + \nabla \quad (5)$$

E_i is actually (within the accuracy of the Hartree approximation) the energy necessary to remove the i -th particle from the nucleus.

In the Hartree-Fock method one uses, instead of the product Eq. (2), an antisymmetrized product, or determinant

$$\Psi = \frac{1}{\sqrt{N!}} \begin{vmatrix} u_1(x_1) & u_1(x_2) & \dots & u_N(x_1) \\ \vdots & \vdots & & \vdots \\ u_1(x_N) & u_2(x_N) & \dots & u_N(x_N) \end{vmatrix}. \quad (6)$$

(It is here implied that spin and isotopic spin variables are contained in these functions, since otherwise we would not deal with a completely antisymmetric function.) The one-particle equations are now:

$$-\frac{\hbar^2}{2m} \nabla^2 u_i(x) - E_i u_i(x) + \int U(x, y) u_i(y) d^3y = 0 \quad (7)$$

where

$$U(x, y) = U(x) \delta(x-y) - \sum_i u_i^*(y) u_i(x) V(x-y). \quad (8)$$

Now $U(x, y)$ is a velocity dependent potential, common to all particles.

The solution of these many coupled equations is troublesome unless we treat small nuclei. However, the approximation should work well only for fairly large nuclei.

As an extreme limit, we can look at large nuclei in the limiting case of uniform nuclear matter. This is possible because the density inside actual nuclei is very nearly uniform. We must in this case, however, switch off the proton-proton Coulomb interaction. We treat each particle as a particle in a box, using cyclic boundary conditions. In this case we find $U(x) = \text{constant}$ for the Hartree potential. Also $U(x, y) = U(x-y)$. The normalized one-particle functions are then

$$u_n = \frac{1}{\sqrt{V}} e^{ik_n x}. \quad (9)$$

The equation for the single-particle functions can be written:

$$(E_n - T_n - U_n) u_n = 0 \quad (10)$$

where U_n is the integral operator:

$$U_n u_n \equiv \int U(x-y) u_n(y) dy^3 . \quad (11)$$

Now we can write:

$$(E' - H'_o) \Psi = 0$$

with

$$E' = \sum_n E_n \quad H'_o = \sum_n T_n + \sum_n U_n .$$

As before,

$$E = \sum_n E_n - \nabla$$

where ∇ is the average mutual potential energy of all the particles. It is convenient to include the constant term $-\bar{V}$ in the definition of the single-particle Hamiltonian, so that the Hartree-Fock value of the ground-state energy is an eigenvalue of this Hamiltonian, without the extra term in Eq. (5). We therefore introduce the Hamiltonian

$$H_o = H'_o - \bar{V} . \quad (12)$$

This may, for example, be achieved by including an extra term $-\bar{V}/N$ in the single-particle potential.

Then

$$(E - H_o) \Phi = 0 \quad (13)$$

has as its lowest eigenvalue the Hartree-Fock energy of the ground state, and as the eigenfunction the Hartree-Fock wave function for the ground state.

If we want to estimate the error of this method, or correct for it, we must use not only the ground state solution of Eq. (13) but also the general solution, say

$$(E_m - H_o) \Phi_m = 0 . \quad (14)$$

Here we are still using the same one-particle potential as in the ground state, Eq. (8), although this is no longer the self-consistent potential for the excited state. This is not likely to make much difference as long as only a few nucleons are excited, and in any case we are not here aiming at a realistic treatment of excited states, but merely at a complete orthonormal set of states for use in perturbation theory.

Now we set up standard perturbation theory on

$$H = H_0 + W \quad (15)$$

where

$$W = (1/2) \sum_{i \neq j} V_{ij} - \sum_i U_i. \quad (16)$$

The importance of higher-order corrections is usually measured by the ratio

$$W/\Delta E \quad (17)$$

where W is some measure of the perturbation Eq. (16), and ΔE is a typical energy difference between the unperturbed states.

It would be wrong to try to get a measure of W by taking its diagonal element for the ground state, since by self-consistency

$$W_{00} = \langle \Psi_0^* W \Psi_0 \rangle = 0.$$

Since this is due to a cancellation, it would be reasonable to use instead the magnitude of each of the terms of Eq. (16) which appear in this diagonal element, which would say that W is about $N\bar{U}$, where \bar{U} is the mean depth of the one-particle well, and N the number of particles.

For ΔE one might take the spacing of the energy levels of a particle in the well. This is

$$\Delta E \sim v \Delta p \sim v \hbar / R$$

where R is a measure of the well radius, and v the nucleon velocity. It would thus appear as if in Eq. (17) the numerator increases and the denominator decreases with the number of particles, so that the errors would be very bad for large nuclei.

We shall see, however, that such an estimate would be misleading. To see this, consider standard perturbation theory:

$$E = E_0 + \epsilon_1 + \epsilon_2 + \dots$$

$$\epsilon_1 = W_{00} (= 0) \quad (18)$$

$$\epsilon_2 = \sum'_n \frac{W_{0n} W_{n0}}{E_0 - E_n}$$

where the prime indicates that we do not sum n over the ground state.

$$\epsilon_3 = \sum_l' \sum_n' \frac{W_{ol} W_{ln} W_{no}}{(E_o - E_l)(E_o - E_n)} - \sum_n' \frac{W_{oo} W_{on} W_{no}}{(E_o - E_n)^2} \quad (19)$$

We must now investigate the higher order terms, in order to see if we ever get contributions proportional to higher powers of N than the first. If we did, of course, the perturbation theory would be useless in the limit of infinite nuclear matter.

Let us first consider ϵ_2 . Remembering that W is a two-particle operator, we see that the only possible transitions are those between states which differ at most in the placing of two particles. Let us now consider only the case where two particles are excited from states α, β to α', β' . Then the matrix element of U , a one-particle operator, vanishes; and we have:

$$\sum_n \frac{W_{on} W_{no}}{E_o - E_n} = \sum_{\alpha, \beta} \sum_{\alpha', \beta'}' \frac{\langle \alpha \beta | V | \alpha' \beta' \rangle \langle \alpha' \beta' | V | \alpha \beta \rangle}{E_\alpha + E_\beta - E_{\alpha'} - E_{\beta'}}$$

If we call the minimum energy denominator ΔE we can write:

$$\epsilon_2 < \frac{1}{\Delta E} \sum_{\alpha \beta} \sum_{\alpha' \beta'}' \langle \alpha \beta | V | \alpha' \beta' \rangle \langle \alpha' \beta' | V | \alpha \beta \rangle .$$

And, using the closure relation we can do the summation over intermediate states, obtaining:

$$\epsilon_2 < \frac{1}{\Delta E} \sum_{\alpha \beta} \langle \alpha \beta | V^2 | \alpha \beta \rangle .$$

Now the sum over α, β is a sum over pairs, and gives rise to $N(N-1)/2$ terms which in the limit of large N is proportional to N^2 . However, since each particle interacts with at most a few neighboring particles, due to the short-range forces, the value of the sum will be only proportional to N .

Now we must also consider the single particle excitations. By exactly the same reasoning we reduce the sum to a sum over the initial states, which are N in number, therefore causing no difficulty. In fact, if W is the self-consistent potential for the interaction V the matrix elements will vanish between the states of one-particle excitation.

Now for ϵ_3 we will again consider the two-particle excitations. Here there are two possibilities. We can excite both particles twice. This leads to no difficulties. However, there is a danger for the case where $l = n$. Now if we are completely self-consistent, the last term

ϵ_3 vanishes because $W_{\infty}=0$. For this case we can eliminate most of the first term also, since W_{11} is almost zero. Our potential is not completely self-consistent for the state l , but since this differs only in the states of two particles, the remainder does not grow with N . However, if we are not completely self-consistent, the last terms will just suffice to cancel the leading terms in the first sum. Therefore, no difficulty is brought on in the third order.

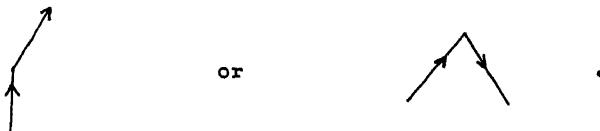
In fourth order we have

$$\begin{aligned} \epsilon_4 = & \sum' \frac{W_{01} W_{1n} W_{nk} W_{k0}}{(E_0 - E_1)(E_0 - E_n)(E_0 - E_k)} \\ & + \left(-2 \operatorname{Re} \sum' \frac{W_{00} W_{01} W_{1n} W_{n0}}{(E_0 - E_1)^2 (E_0 - E_n)} + \sum' \frac{W_{00}^2 W_{0n} W_{n0}}{(E_0 - E_n)^3} \right) \quad (20) \\ & - \left(\sum_n \frac{W_{0n} W_{n0}}{E_0 - E_n} \right) \left(\sum_n \frac{W_{0n} W_{n0}}{(E_0 - E_n)^2} \right) . \end{aligned}$$

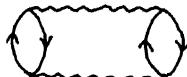
The terms which really give trouble here are the ones in which we excite first one pair, and then another, and then return both to their original states. Now, in the self-consistent theory, the terms with $W_{\infty\infty}$ vanish, but the last term remains. It can be shown that this term just cancels the terms in the first summation which correspond to exciting two pairs independently.

J. Goldstone¹ has shown that this cancellation occurs in all orders of perturbation theory. We shall just sketch his method here. He uses a graphical method, not unlike the Feynman diagrams of field theory.

Each occupied state outside the states occupied in the ground-state configuration is indicated by an arrow going up, and each vacancy is denoted by an arrow going down. Then the two possible situations are



Clearly, the lines will always be closed. Each two-particle interaction is shown by a wavy line connecting two vertices. Therefore, the simplest diagram we can have may be denoted as



second order.

In third order we may have



Now in fourth order we may have "unlinked clusters," described, for example, by



Goldstone shows that there is a one-to-one correspondence between his graphs and the terms in perturbation theory. What Goldstone then shows is that the contribution of the unlinked clusters all cancel out, and that unlinked diagrams may be omitted from the start.

Another way of judging the applicability of perturbation theory is to examine the wave function. The usual reasoning implies that the new wave function should not differ very much from the old one. We have

$$\Psi_0 = \phi_0 + \sum_n' \frac{W_{n0}}{E_0 - E_n} \phi_n = \phi_0 + \Psi \quad (21)$$

where we are only considering the first-order corrections to the wave function. We should have $\Psi \ll \phi_0$. Let us consider:

$$\int |\Psi|^2 dx = \sum_n \frac{|W_{n0}|^2}{(E_0 - E_n)^2} .$$

By the same consideration as used in the second order perturbation term to the energy, we see that we get a term proportional to N .

The question which naturally presents itself is that if

$$\int |\Psi|^2 dx$$

is proportional to N , why is it that we obtain good results for large N ? The reason for this is most easily seen by way of a simplified example. Consider the case in which the perturbation is due to an external force on each particle, instead of a two-body force: $H = H_0 + W$ where $W = \sum_i \omega(x_i)$ a sum of one-particle operators.

Let us further assume that the particles are bosons, and that the Pauli exclusion principle does not hold. Then we can start with all our particles in the ground state and write:

$$u'_\alpha = u_\alpha + \sum'_\beta \frac{\omega_{\beta\alpha}}{\epsilon_\alpha - \epsilon_\beta} u_\beta$$

and

$$\Psi = \prod_i [u_o(x_i) + \sum'_\beta \frac{\omega_{\beta o}}{\epsilon_o - \epsilon_\beta} u_\beta(x_i)].$$

If we expand this product into a sum, and keep only two terms, we find

$$\Psi = \phi_o + \sum_i \sum_\beta \frac{\omega_{\beta o}}{\epsilon_\beta - \epsilon_o} \frac{u_\beta(x_i)}{u_o(x_i)} \phi_o$$

which is identical with Eq. (21). Because of the summation over i , this term is proportional to N , and the expansion is evidently not legitimate. However, we can obtain a reasonable approximation by writing

$$\Psi = \phi_o \exp \left[\sum_i \sum'_\beta \frac{\omega_{\beta o}}{\epsilon_o - \epsilon_\beta} \frac{u_\beta(x_i)}{u_o(x_i)} \right]. \quad (22)$$

Thus we should think of the perturbation series as occurring in the exponent, rather than in the wave function itself. It is possible to work with an approximate wave function of such an exponential form, but the calculations then become unwieldy.

Instead, we may note that all physical quantities of interest can be expressed in terms of one-and two-particle density matrices. The one-particle density matrix is defined by

$$Q_1(x_1; x'_1) = \frac{\int \Psi(x_1, x_2, \dots, x_N) \Psi^*(x'_1, x_2, \dots, x_N) dx_2 \dots dx_N}{\int |\Psi|^2 dx_1 \dots dx_N}. \quad (23)$$

From this, we can, for example, obtain the kinetic energy as

$$T_1 = - \frac{\hbar^2}{2m} \int \left[\frac{\partial^2 Q_1(x_1, x'_1)}{\partial x_1^2} \right]_{x'_1=x_1} dx_1.$$

Similarly the two-particle density matrix is

$$\rho_2(x_1, x_2; x'_1, x'_2) = \frac{\int \Psi(x_1, x_2, x_3, \dots, x_N) \Psi^*(x'_1, x'_2, x_3, \dots, x_N) dx_3 \dots dx_N}{\int |\Psi|^2 dx_1 \dots dx_N} \quad (24)$$

from which we find the mutual potential energy

$$V_{12} = \int V(x_1 - x_2) \rho_2(x_1, x_2; x'_1, x'_2) dx_1 dx_2.$$

In our case the one-particle matrix is seen to be from Eq. (22):

$$\frac{\left[u_o(x_1) + \sum' \frac{w_{\alpha\beta}}{\epsilon_o - \epsilon_\alpha} u_\beta(x_1) \right] \left[u_o(x'_1) + \sum' \frac{w_{\alpha\beta}}{\epsilon_o - \epsilon_\alpha} u_\beta(x'_1) \right]^*}{\int |u_o(x_1)|^2 dx_1 \int |u_o(x'_1)|^2 dx'_1}$$

in which the correction terms are independent of N. The same is true of the two-particle density matrix.

In the realistic case in which the perturbation consists of two-body interactions rather than an external potential the perturbed wave function no longer factorizes exactly, but it is still true that the density matrices can be expanded in series in which no positive powers of N appear.

In other words, the kinetic and potential energies which can be expressed in terms of one- and two-particle density matrices are perturbed only to the extent to which the perturbation affects the motion of one or two particles, and in a reasonable model this effect does not grow with N. This argument, which is another way of expressing the reasoning used by Goldstone, is taken from work by J. Lascoux at Birmingham.

We see, therefore, that the numerator to use in our criterion Eq. (17) does not, in fact, grow with N. Next consider the denominator in connection with the danger that the occurrence of matrix elements between adjacent states, with small denominators, might still ruin perturbation theory.

Here we are greatly helped by the Pauli principle. If we consider one- or two-particle transitions involving particles in the lower occupied states in the Fermi distribution, Eq. (6), then no transition is possible in which these particles change their energy only by a small amount, since all adjacent states are already occupied. Hence the only transitions involving such particles have energy denominators of a magnitude comparable to the Fermi energy.

This is not true for the particles in the highest occupied states, which can make transitions to empty states with a small change of energy. Here we are really dealing with small denominators, and the behaviour

of these particles near the edge of the Fermi distribution is probably not given correctly by perturbation theory. Because of the small number of such particles, this complication is not likely to be important for the overall effects, such as the total binding energy of the nucleus. For finer dynamical effects, such as the nature of low-lying excited states, it may be important. These effects, which we shall neglect here, have been studied recently by Bohr, Mottelson and Pines² and by Belyaev.³

We expect, therefore, that for the calculation of binding energy and other overall effects, the Pauli principle will prevent the occurrence of small energy denominators except in a few terms.

This importance of the Pauli principle means that it is of practical importance to conduct the calculations in such a way that transitions forbidden by the Pauli principle are excluded from the beginning. This is not forced upon us by the mathematics of the calculation. Consider, for example, a term of second order in the energy

$$\sum' \frac{|W_{on}|^2}{E_o - E_n} .$$

The summation is over all excited states of the non-interacting particles. Here only symmetric states count, but we may also extend the summation over states of all symmetry, since for a symmetric interaction W the matrix element W_{on} vanishes unless the state n has the same symmetry as the initial state O , i. e., is antisymmetric. Summing over all states of any symmetry is, however, equivalent to summing independently over the states of individual particles.

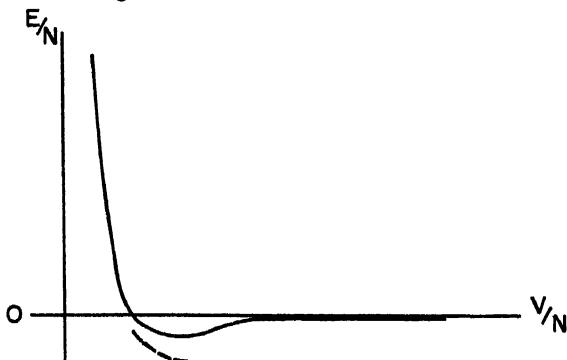
In this form one therefore includes transitions which violate the Pauli principle, but their contribution to the result must, of course, cancel out in the end. If we proceeded in this way, however, each term in our perturbation series would appear as a small difference between large terms, and this would obscure its significance, and might cause errors if each term is not evaluated to a high accuracy.

Let us now turn to a more quantitative discussion of the case of uniform nuclear matter. In that case the Hartree-Fock potential will be independent of space but dependent on the velocity. $U(x, y)$ in Eq. (8) will be a function of $x-y$ only. The velocity dependence of the single-particle potential then depends on the exchange nature of the two-body force. We shall assume a mixture of "ordinary" forces with a potential $V(r)$ and "exchange" forces with an energy $(-1)^l V(r)$, where l is the mutual orbital angular momentum of the two interacting nucleons. If we are to have saturation, i. e., if we wish to avoid the collapse of heavy nuclei, the exchange part must not be too small (cf. Blatt and Weisskopf, p. 140 et seq.).

In addition, there are tensor forces contained in the two-body interaction. However, these do not contribute much to the binding energy of a large nucleus and we may therefore disregard them for the present

purpose.

A perturbation calculation of this type was done by Euler as early as 1937.⁴ He calculated the energy as a function of the volume per particle, and hence the equilibrium density, compressibility, and binding energy. For infinite nuclear matter one determines one's wave functions by cyclic boundary conditions, and these fix the volume per particle which therefore enters the calculations as a parameter. Euler used saturating forces with a Gaussian dependence on distance. His results were, qualitatively, as shown in Fig. 1.



X Fig. 1

The binding energy per particle is shown against the volume per particle. The full curve is the energy in the Hartree-Fock approximation, the cross indicates the experimental result, and the broken curve the calculation to second order.

While the second-order correction is comparable with the unperturbed binding energy, one must remember that this is a small difference between a large potential energy and a large kinetic energy. The correction is therefore quite small in relation to the quantities which are being corrected, and might indicate that the approximation is working well. However, at the time Euler's result was generally taken to mean that the basic Hartree-Fock approach was bad, and that perturbation theory would converge badly. There are three reasons for this:

In the first case, if perturbation theory was applicable, then the model gave results in disagreement with experiment, and therefore the forces used must be wrong. It was, however, believed at the time that forces of this type were correct.

A stronger reason came from the fact that the forces assumed by Euler were capable of accounting well for the binding energy of the α particle. For a system of $N/2$ neutrons and $N/2$ protons, they should therefore give a ground-state energy at least as low as that of $N/4 \alpha$

particles. These have a binding energy which is a large fraction of the observed binding energy of the N -particle nucleus, and much larger than Euler's value. Hence Euler's approximation to the ground state of the nucleus could not be right.

The answer to this objection is that the argument predicts only the energy of separated α particles, for which a large volume is required. In nature we know that α particles attract each other, but it does not follow that they do so under the forces postulated by Euler; and, if they don't, the correct curve in the figure, while as low as the cross at very large volumes, may lie close to Euler's value near the normal density. Thus Euler's calculation would be correct near normal density but would be a bad approximation for much lower density.

This is precisely what we might expect from the importance of the Pauli principle for the convergence of perturbation theory. At lower density the kinetic energy of the Fermi gas is less and with it the effectiveness of the Pauli principle in increasing the energy denominators.

A third reason for suspecting Euler's answer was based on the fact that in the two-body problem perturbation theory, which starts from the wave function for non-interacting particles gives a very poor approximation.

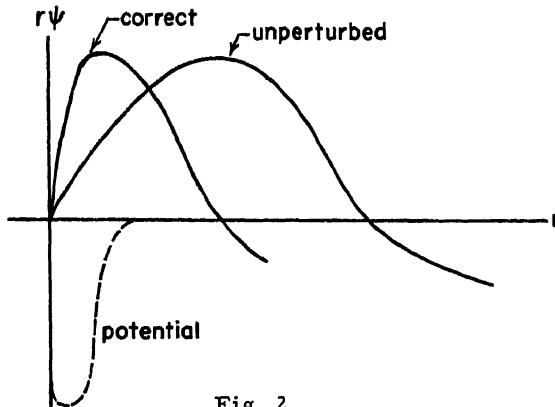


Fig. 2

Fig. 2 shows the correct and the unperturbed wave functions for two nucleons. Although their difference is not large, it is appreciable in the region where the potential acts. The average potential energy depends on

$$\int V(r) (r\psi)^2 dr$$

for which the unperturbed wave function is very poor. The same, it seemed, should apply inside a large nucleus if, as in Hartree or Hartree-Fock, we estimate the interaction by taking the particles as moving inde-

pendently from each other.

This argument, too, ignored the Pauli principle. The distortion of the wave function by the forces represents an admixture of other unperturbed states. In so far as these are occupied states, this must be compensated by a reduction of the extent to which other particles are found in these states. In other words, if the forces result in drawing a particular particle closer to a given one, the Pauli principle ensures that others will be kept further away. For the calculation of the total energy these contributions cancel, and the result is the same as if the admixture to a given wave function of normally occupied states were left out.

The same point can be made by saying that the effect of the distortion on the interaction represents the change in the density of the nucleon gas in the presence of a given nucleon. This depends on the compressibility of the gas, and it is well known that a Fermi gas is much less compressible than a classical gas.

We see, therefore, that the discrepancy between Euler's result and the true nuclear energy is not due to a failure of his approximation, and must therefore depend on the assumed forces. It is not due to the detailed Gaussian shape, since a later calculation by Huby, with Yukawa type forces, gave substantially the same result.

But if we alter the exchange mixture and include less exchange force we can get much more binding for a large nucleus. Originally the idea of exchange forces had been introduced as a speculation by Heisenberg, in order to account for saturation. More recently, experiments on neutron-proton scattering at energies of a few hundred Mev have given direct evidence of exchange forces.

At such energies the wavelength is much less than the range of the forces; so one expects the momentum transfer between the particles to be small compared to their relative momentum, and hence the scattering angle should be small. The experiments indeed show a large peak at small scattering angles, but also another peak at 180 degrees in the center-of-mass system. This is easily understood if there are exchange forces, since they result in the particles exchanging their places, so that the particle travelling nearly in the forward direction has become the proton, and the recoiling one is the neutron. From the equality of the forward and backward peaks one concludes that the forces consist in equal parts of ordinary and exchange forces, and such a mixture does not saturate, but would give a much stronger binding energy than the saturating mixture assumed by Euler.

Hence the same experiments which confirmed our belief in the existence of exchange forces, showed that they were inadequate to meet the need for which they had been invoked, and there must be some other factor tending to produce saturation.

Besides exchange forces, the following effects may produce saturation:

Repulsive forces at short distances ("repulsive core") which are the main reason for the finite density of ordinary solids and liquids.

Many-body forces. These may be expected to be repulsive, and would then act, qualitatively, like repulsive cores.

Velocity dependent forces. If the mutual attraction between two particles diminishes as their relative velocity increases, this will work against a collapse, since with increasing density all kinetic energies, and hence also the relative velocities, go up. We shall see that the effect of this is very similar to that of a repulsive core.

The phase shift analysis of proton-proton scattering data at about 300 Mev⁵ has shown that the ¹S phase shift is negative at these energies. Negative phase shifts suggest a repulsive interaction, and since at lower energies the phase shift is positive, there must be some attraction and some repulsion present. An attractive potential with a strong repulsive core would give a phase shift which goes from positive to negative values as the energy increases.

(One could, of course, obtain the same result from a velocity dependent potential which is purely attractive at low energy and purely repulsive at high energy.)

If one interprets the experiments in terms of a repulsive core, its width is rather small ($\sim .4$ fermis). Therefore, in order to give appreciable repulsion it must be very high.

The strong repulsive core leads to severe difficulties in the Hartree approximation. The use of perturbation theory with such a large potential will give terms so large that there is no hope of arriving at a convergent result. Since this is the case, we may as well assume that the core is infinite.

It was principally Brueckner who figured out how to adapt perturbation theory to this situation. Essentially, he makes use of the fact that we can solve the problem exactly for the two-body case. The basic method here is a generalization of one developed by Watson⁶ for high-energy problems.

Our presentation will follow that of Tobocman.⁷ One of the best papers to read in order to gain insight into the problem is a paper by H. Bethe.⁸ Brueckner has a whole series of papers on the subject, and we refer here only to one of the later ones, which contains references to his earlier papers.⁹

We start with the Hamiltonian:

$$H = \sum_i^N T_i + \sum_{i>j} V_{ij} .$$

We assume, of course, that we can solve the independent-particle problem, with

$$H_0 = \sum_i^N T_i + \sum_i U_i .$$

We note here that U_i may be velocity dependent. We denote the ground

state solution of H_0 by ϕ_0 and of H by ψ_0 . Also we write $E - E_0 \equiv \Delta$ then

$$\begin{aligned}\Delta &= \frac{\langle \phi_0 | H - H_0 | \psi_0 \rangle}{\langle \phi_0 | \psi_0 \rangle} \\ &= \frac{\langle \phi_0 | V - U | \psi_0 \rangle}{\langle \phi_0 | \psi_0 \rangle}.\end{aligned}$$

We write this as

$$\Delta = \langle \phi_0 | (V - U) \Omega | \phi_0 \rangle$$

where

$$\Omega \phi_0 = \frac{\psi_0}{\langle \phi_0 | \psi_0 \rangle}.$$

Now we find the equation for Ω , obtained from the equations for ϕ_0 and ψ_0 :

$$\Omega = 1 + G(V - U - \Delta)\Omega$$

where

$$G = \frac{1}{E_0 - H_0}(1 - P)$$

where P is a projection (25) operator.

$$P = |\phi_0\rangle\langle\phi_0|$$

The factor $(1 - P)$ is inserted to avoid those terms for which the denominator vanishes (eigenstates of H_0 with eigenvalue E_0). Now we can expand Ω in an infinite series. Now clearly we cannot use this expression in the equation for Δ because it contains V , which is infinite in the region of the core.

Let us digress a moment and discuss the two-body problem. We define the two-body scattering matrix t as follows:

$$t = V + V g t$$

where g is a suitable two-body Green's function. (26)

For the moment we shall not specify g , but leave it arbitrary. Now we write

$$t = V\omega$$

where ω is the wave matrix of the two-body problem and a solution of the equation:

$$\omega = 1 + gV\omega.$$

We may now use the expression which defines t in order to write V as a power series in t . That is

$$\begin{aligned} V &= t - Vgt \\ &= t - tgt + tgtgt - \dots \end{aligned} \tag{27}$$

Now what we shall do is to insert this series expansion in the expression for Δ in the many-body problem. Whether or not this series converges is still a question, of course. We shall label the two-body operator by α which will represent pairs of particles. Then we have

$$V = \sum_{\alpha} V_{\alpha} \quad V_{\alpha} = t_{\alpha} - t_{\alpha} g_{\alpha} t_{\alpha}.$$

Now we can write Δ in the following form:

$$\begin{aligned} \Delta &= \langle Q_1 \rangle + \langle Q_1 G Q_1 \rangle + \langle Q_1 G Q_2 G Q_1 \rangle + \dots \\ &\quad + \langle Q_2 \rangle - \langle Q_1 \times Q_1 G G Q_1 \rangle - \dots \\ &\quad + \langle Q_1 G Q_2 \rangle + \dots \end{aligned} \tag{28}$$

where we write

$$V - U = \sum_{n=1}^{\infty} Q_n.$$

If we write

$$Q_1 = V - U \quad Q_2 = Q_3 = \dots = 0$$

we get the ordinary perturbation series expansion:

$$\Delta = \langle V - U \rangle + \langle (V - U) G (V - U) \rangle + \dots$$

We can also build up a different series using the expansion Eq. (27) of ∇ in terms of t :

$$Q_1 = \sum_{\alpha} t_{\alpha} - U \quad Q_2 = - \sum_{\alpha} t_{\alpha} g_{\alpha} t_{\alpha} \quad Q_3 = \dots$$

Then we get a perturbation series of the form

$$\begin{aligned} \Delta = & \left\langle \sum_{\alpha} t_{\alpha} - U \right\rangle + \left\langle (\sum_{\alpha} t_{\alpha} - U) G (\sum_{\alpha} t_{\alpha} - U) \right\rangle + \dots \\ & - \left\langle \sum_{\alpha} t_{\alpha} - U \right\rangle \times \left\langle (\sum_{\alpha} t_{\alpha} - U) G G (\sum_{\alpha} t_{\alpha} - U) \right\rangle + \dots \quad (29) \\ & - \left\langle \sum_{\alpha} t_{\alpha} g_{\alpha} t_{\alpha} \right\rangle . \end{aligned}$$

Finally we may define an operator T such that

$$T_{\alpha} = (V_{\alpha} - U_{\alpha}) + (V_{\alpha} - U_{\alpha}) g_{\alpha} T_{\alpha} ;$$

then we can define:

$$Q_1 = \sum_{\alpha} T_{\alpha} \quad Q_2 = \sum_{\alpha} T_{\alpha} g_{\alpha} T_{\alpha} .$$

Here U_{α} is defined as a sum of two one-body operators such that

$$\sum_{\alpha} U_{\alpha} = U = \sum_i U_i .$$

We still have g_{α} at our disposal. We shall want to choose this in such a way as to bring about cancellation of the higher-order terms. This will then improve the result of lowest order, namely

$$\left\langle \sum_{\alpha} t_{\alpha} - U \right\rangle .$$

Let us consider the following higher order terms:

$$\begin{aligned} & \left\langle (\sum_{\alpha} t_{\alpha} - U) G (\sum_{\alpha} t_{\alpha} - U) \right\rangle \\ & - \sum_{\alpha} \left\langle t_{\alpha} g_{\alpha} t_{\alpha} \right\rangle . \end{aligned}$$

Now we could let

$$g_{\alpha} = G_{\alpha} .$$

However, we note that the latter term does not take the Pauli principle

into consideration at all. We can take the Pauli principle into account in an approximate way by writing

$$g_\alpha = G_\alpha(1 - Q) ,$$

where Q is a projection operator which projects out the states of the Fermi sea. The effect of $(1 - Q)$ then is to eliminate scattering into any of the states normally occupied in the ground state. Clearly in terms of high order, when many particles are excited, this is not a good approximation. However, we do not have to worry about this too much, since if these terms are at all important, then our perturbation theory is doomed to fail anyway.

The scattering problem with a hard core, taking the Pauli principle into account, was worked out by Bethe and Goldstone.¹⁰

We can write the Schrödinger equation for two particles as

$$\frac{\hbar^2}{2m}(\nabla_1^2 + \nabla_2^2)\Psi + E\Psi = V\Psi .$$

We can write the right-hand side in the following way:

$$V\Psi = \sum_{m,n} \langle u_m^*(r_1) u_n^*(r_2) V(r_1 - r_2) \Psi(r_1, r_2) \rangle u_m(r_1) u_n(r_2) .$$

Now it is clear what we must do. In order to avoid scattering into states in the Fermi sea we must restrict the summation over m and n to states with $m, n > k_F$ where k_F labels the highest state of the Fermi sea.

We may now write down the scattering equation excluding occupied states as intermediates. We obtain

$$\frac{\hbar^2}{2m}(\nabla_1^2 + \nabla_2^2)\Psi + E\Psi = V\Psi - \sum_{\substack{m \leq k_F \\ n \leq k_F}} \langle u_m^* u_n^* V\Psi \rangle u_m u_n .$$

We shall restrict ourselves in what follows to the case of uniform nuclear matter. Here actually there is a constant (in space) potential, which appears in the Hamiltonian, and can merely be lumped into the constant E . The right-hand side now becomes

$$V(r_1 - r_2)\Psi - \frac{1}{(2\pi)^3} \int_{k_1, k_2 < k_F} e^{ik_1(r_1 - r_1') + ik_2(r_2 - r_2')} V(r'_1, r'_2) \Psi(r'_1, r'_2) d^3 k_1 d^3 k_2 dr'_1 dr'_2 .$$

Now making the substitution

$$\frac{1}{2}(r_1 + r_2) = R$$

$$r_1 - r_2 = r$$

we then obtain

$$\begin{aligned} \frac{\hbar^2}{4m}\nabla_R^2\Psi + \frac{\hbar^2}{m}\nabla_r^2\Psi + E\Psi &= V(r)\Psi - \\ -\frac{1}{(2\pi)^3}\int d^3R'd^3r'e^{i(k_1+k_2)(R-R')}e^{\frac{i}{2}(k_1-k_2)(r-r')}V(r)\Psi(R,r')d^3k_1d^3k_2. \end{aligned} \quad (30)$$

The equation simplifies if we write

$$\Psi = e^{iP \cdot R} \phi(r).$$

Then we have

$$-\frac{\hbar^2}{4m}P^2\phi + \frac{\hbar^2}{m}\nabla^2\phi + E\phi = V(r)\phi - \frac{1}{(2\pi)^3}\int d^3Kd^3r'V(r)e^{iK(r-r')}.$$

Here we have done the integration over d^3R' , which is trivial, and changed variables such that

$$k_1 = \frac{P}{2} + K \quad k_2 = \frac{P}{2} - K.$$

Note now that the integration over K is not over a spherical region, but over the intersection of two spheres. If we take the case $P=0$, then the integration is just the integral over a sphere again, and we shall consider this case in detail. Then the equation is separable in polar coordinates. We shall only consider S-wave scattering, since that is the only important case when there is a hard core. We write $r\phi=u$ and take $l=0$; then the equation becomes:

$$\frac{\hbar^2}{m}\frac{d^2u}{dr'^2} + (E - V)u = \int K(r,r')V(r')dr' \quad (31)$$

where $K(r,r')$ may be determined from the previous equation.

In order not to complicate the problem, we shall just consider a repulsive core potential and ignore the attractive well.

$$\nabla = \infty \quad r < a$$

$$\nabla = 0 \quad r > a$$

Then clearly $u=0$ for $r < a$. However, we still have the term ∇u in the equation, which is indefinite for $r < a$, since $u=0, \nabla=\infty$. Let us define $\omega = \nabla u$. Then $\omega=0$ for $r>a$. Consider the equation at the point $r=a$. The slope of u will in general be finite at a . Let us write

$$b = \left(\frac{du}{dr} \right)_{r=a}. \quad (32)$$

Clearly, the slope is zero for $r < a$. Therefore, we see that there is a singularity in the second derivative at the point a . This is of the nature of a delta function. Then, considering the equation at $r=a$ we can write:

$$\frac{\hbar^2}{m} b \delta(r-a) - \omega(a) = \int K(a, r') \omega(r') dr'. \quad (32)$$

The integral must be a smooth function, without singularities. Therefore, the singularity must be attributed to ω . We write:

$$\omega = \frac{\hbar^2}{m} b \delta(r-a) + \omega_1$$

where ω_1 is the non-singular part of ω . When we consider the equation for $r < a$, we obtain:

$$-\omega_1 = \int K(r, r') \omega(r') dr' + \frac{b\hbar^2}{m} K(r, a).$$

Bethe and Goldstone show that the major part of ω_1 is

$$\frac{b\hbar^2}{m} K(r, a)$$

and that we get a rapidly convergent result if we solve this equation by iteration; i. e.,

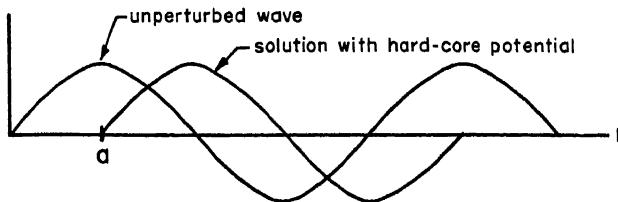
$$\omega_1 = - \frac{b\hbar^2}{m} K(r, a) + \int K(r, r') \left[-\frac{b\hbar^2}{m} K(r', a) \right] dr' + \text{etc.},$$

which turns out to give a power series in $(a^3 k_F)$. This is made rapidly convergent by the favorable numerical factors brought in by the integrations. Now we can write the equation for $r > a$:

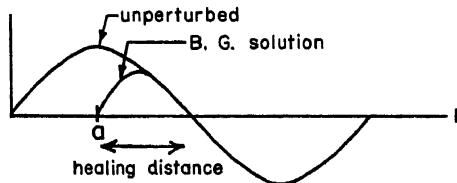
$$\frac{\hbar^2}{m} \frac{d^2 u}{dr^2} + Eu = \int_0^a K(r, r') \omega(r') dr'. \quad (33)$$

The integration over r' is cut off at a , since $\omega = 0$ for $r > a$. The resultant equation is now a typical inhomogeneous equation, whose solution provides no difficulty. Let us see what we get.

For the S wave, the ordinary Schrödinger equation would give the following solution:



The solution to the Bethe-Goldstone equation looks like this:



Since scattering is determined by the phase shift and transitions are forbidden, then we obtain a wave function which in Weisskopf's expression is "healed" after a short distance.

Now let us return to the many-body problem. The first two terms in the expansion for Δ were:

$$\left\langle \sum_{\alpha} t_{\alpha} - U \right\rangle + \left\langle \left(\sum_{\alpha} t_{\alpha} - U \right) G \left(\sum_{\alpha} t_{\alpha} - U \right) \right\rangle.$$

We have already shown how the terms in the second expression could be cancelled by

$$\left\langle \sum_{\alpha} t_{\alpha} g_{\alpha} t_{\alpha} \right\rangle$$

when we considered two body excitations. However, we still have to consider the excitations involving one particle, and the diagonal terms (corresponding to no excitation). The zero-and one-particle excitations may

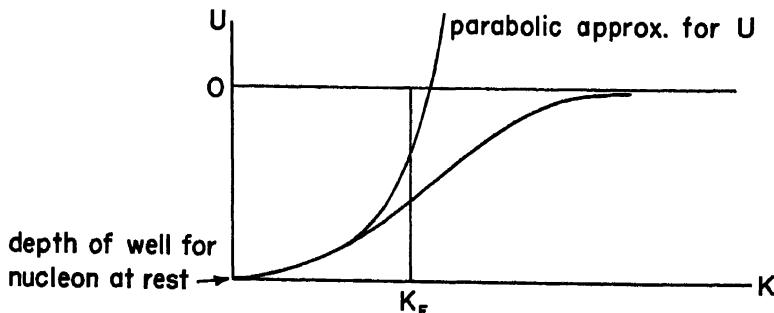
be eliminated by the use of a self-consistent potential. We define:

$$U_i = \sum_j \int \phi_j^* t_{ij} \phi_j d^3 r_j + \text{exchange terms} .$$

Now it is clear that U_i is a momentum dependent operator, since t_{ij} is momentum dependent. U_i will be an attractive potential which will become weaker for higher momentum. We can see this in two ways. First, the exchange terms, which are a measure of the overlap of the wave functions, will decrease for particles well above the edge of the Fermi sea. Furthermore, the effect of the repulsive core becomes more noticeable for high momentum transfer. Therefore, the net effect is to decrease the attractive force in the high momentum region.

We may digress for a moment and notice that the Pauli principle, the exchange terms, and the repulsive core all give the same qualitative result, i. e., decreasing attraction at high momentum. Even if we have interpreted the change of sign of the S phase wrongly in terms of a repulsive core and it is instead due to a velocity-dependent potential, our conclusions would, qualitatively at least, remain the same.

Now let us make a plot of the potential U as function of the wave-vector K .



If we want to use a self-consistent procedure, the momentum dependence of U must be allowed for in the propagator g which is used in the definition of the two-body scattering matrix t . This means that in the Bethe-Goldstone equation we must allow for the presence of a velocity dependent one-particle potential. This complicates the calculation, but there is a special case which can be handled without any additional complication.

This is to expand the potential U into powers of the momentum:

$$U = U_0 + AK^2 + \dots$$

If we stop at the parabolic term, we may write

$$H_0 = U_0 + \frac{\hbar^2}{2m^*} k^2 \quad (34)$$

where m^* is an effective mass, which combines the effect of the momentum dependence of the potential with kinetic energy. Since A is positive (the attraction is less and thus the potential rises as the momentum increases), m^* is less than the real nucleon mass m . Brueckner's calculations show that m^* is appreciably less than m .

However, it must be remembered that we are using the value of the Green's function g only for virtual states and that, because of the way in which we have allowed for the Pauli principle, only virtual states outside the Fermi sea enter. In this region the parabolic approximation may be very bad.

An equally simple device, which would probably give a better approximation, is to take the potential as constant for the intermediate states, i. e., use the normal nucleon mass in the Bethe-Goldstone equation, but to allow the correct energy value of the initial state which in solving the equation is kept constant, so that it need not be expressed in analytical form. As far as I am aware, this possibility has not yet been explored in detail.

A more exact, but also much more laborious procedure is to use a general function $U(k)$, so that the Bethe-Goldstone equation becomes an integral equation, which can be handled by electronic computing techniques. The integration over intermediate states is replaced by a summation, by dividing the momentum into small intervals, and the value of the potential energy for each momentum interval is given numerically. After determining the t -matrix and thus obtaining the diagonal elements, a new function $U(k)$ is determined and the process repeated with this, until the potential is "self-consistent."

Such a calculation was done by Brueckner and Gammel.¹¹ The two-body interaction they assumed was taken from the work of Gammel and Thaler,¹² who had fitted the Berkeley data on p-p and n-p scattering by phenomenological potentials. The Brueckner-Gammel calculations were actually started using the earlier potential fitted by Gammel, Christian and Thaler,¹³ which had given a reasonably good fit for the scattering cross sections, but could not account for polarization measurements. The potential used here was always of the Yukawa type, i. e., of the form

$$A \frac{e^{-kr}}{kr}$$

but with a hard repulsive core superimposed; the strength and range parameters, A and k , and the core radius were adjusted separately for each orbital, spin and charge state.

The Gammel-Thaler potential differs by including also a spin-orbit

coupling, which allows one to obtain agreement also with the polarization data. In this case it turns out that one may choose the core radius to be the same in all states, about 0.4 fermis.

The results of Brueckner and Gammel were then adjusted, in the light of this development, so as to correspond approximately to the new Gammel-Thaler potential.

By calculating the energy per nucleon as a function of density and looking for its minimum, one obtains the binding energy of nuclear matter and its equilibrium density. The figures were about 14 Mev per nucleon, and a density corresponding to a radius $r_0 = 1.07$ fermis per nucleon. Both figures are in good agreement with experiment. They should not be compared directly with the binding energies or the radii of large nuclei, because of the Coulomb repulsion, but one must use the semi-empirical mass formula to separate purely nuclear volume effects from surface and Coulomb effects.

A highly idealized, but instructive, calculation has been done by Gomes, Walecka, and Weisskopf.¹⁴ They use a hard core with a square well attractive potential. They take zero interaction for the odd angular momentum states, and an attractive interaction for the even states, in order to take exchange into account. The simplicity of this calculation allows one to avoid extensive numerical work, and thus brings out the physical significance of the method more clearly.

One serious question remains, however. That is, are the higher order terms, which we have neglected, really negligible? The only way this question can really be answered is by actual calculation of the higher-order terms. This, of course, is a formidable undertaking. P. Martin and De Dominicis have done some work on this problem. Their method was to use a potential which would fit the two-body data, and be easy to handle mathematically. A velocity-dependent potential can be written in the following manner:

$$\nabla \Psi = \int K(r, r') \Psi(r') dr' .$$

If the potential is an ordinary potential we have

$$K(r, r') = \delta(r - r') V(r') .$$

Now what Martin and De Dominicis assumed was that $K(r, r')$ could be written as $f(r)f(r')$, a device first used by Yamaguchi. This is certainly an unphysical assumption, made solely for convenience. Then the function $f(r)$ was chosen to fit the low-energy two-body data. This can evidently be done, since in the low energy region the kinetic energy does not vary very much, and so the velocity dependence is unimportant. One might, however, expect that the velocity dependence implied by this separable potential would give very wrong results at higher energy. It turned out, rather surprisingly, that the qualitative behaviour still remains good,

for example, the 1S scattering phase changes sign just about at the energy at which it does so experimentally.

Using this separable potential, Martin and De Dominicis were able to carry the calculation to the next order and found that the corrections were reasonably small. They pointed out, in this connection, that it is not necessary to take the requirement of self-consistency too literally. Since in any event there remain correction terms, it is sufficient to satisfy self-consistency to a point at which the first-order corrections (which would vanish for complete self-consistency) are of the order of the second-order corrections.

We see therefore that, although much remains to be done, these developments have led, for the first time, to a situation in which we start with something like the real two-body forces and come out with the correct picture of nuclear matter, in a spirit very close to that of the shell model.

For a quantitative justification of the shell model, it is, of course, not sufficient to apply the method to uniform nuclear matter, but we must consider the problem of a finite nucleus. This presents us with two new difficulties, one practical and one of principle.

The first arises from the question how one is to carry through the calculations for a finite nucleus, assuming that the approximations work equally well. In the spirit of the method we have sketched, one starts from the eigenfunctions in a potential well, which again will be velocity-dependent. One must then determine the t matrix, which describes the mutual scattering of two particles in this well (and under the influence of the Pauli principle arising from the presence of other particles). Such a matrix must refer to the initial and final quantum states of the two particles, i. e., be of the form

$$\langle n_1, n_2 | t | n'_1, n'_2 \rangle$$

and even to write down such a matrix when it is known is a formidable problem. The trouble is that we have lost here the conservation of momentum, which helped to simplify the t matrix in the case of uniform nuclear matter. This trouble would be less serious in a very light nucleus in which the number of quantum states to be considered is small. However, the spirit of the whole method (as that of the shell model) applies only to reasonably large numbers of particles, and it is doubtful whether one can expect much use from the method for nuclei lighter than, say ^{16}O .

It has been suggested that one might treat the potential as slowly varying, so that the nucleon-nucleon collisions could be assumed to be taking place in a locally constant potential. In that case one might use the t matrix for infinite nuclear matter, but for a density appropriate to the point at which the collision takes place. However, in the surface region (and, after all, the surface is what distinguishes a finite from an infinite nucleus) the density varies so rapidly that it is most doubtful

whether this approximation makes any sense.

But, apart from this difficulty of evaluation, it is also not obvious that the whole method of expansion would still be satisfactory for a finite nucleus. We had seen earlier the important role which the Pauli principle played in the convergence of the expansion. Now the effectiveness of the Pauli principle depends on the density, and in the surface region the density is reduced. This may well mean that near the surface the forces between nucleons have a greater effect on their motion than in the interior. This would apply more to the attractive forces, since the repulsive core, which is of short range, acts mostly through large momentum transfer and therefore is not much reduced by the Pauli principle.

This conjecture receives some support from some experimental facts. One of these relates to the decay constants of α -radioactive nuclei. This can be expressed in the form

$$b e^{-G}$$

where G is the well-known Gamow barrier penetration factor, and b is a quantity of the dimension of an inverse time, which represents the rate at which α particles hit the inside of the barrier.

Now if the picture of independent nucleons with only weak correlations, which we have found useful for uniform nuclear matter were valid up to the surface, we should expect the probability of four nucleons being in the right configuration and of suitably small relative velocity to form an α particle quite small. On the other hand, the empirical decay constants seem to agree well with b being of the order of the inverse radius of the nucleus divided by the α -particle velocity.

A similar argument can be based on recent experiments by P. E. Hodgson, in which the bombardment of nuclei by protons was shown to produce "knock-on" α particles. The yield of this reaction, together with the known cross section for the elastic scattering of protons by α particles suggests that the number of α particles to be found in the nucleus is much larger than one would guess from the shell model. Since only α particles near the surface have a reasonable chance of escaping, this again indicates that the nuclear surface contains nucleons combined into α particles, and thus strong correlations.

Some work is now going on at Birmingham to study the effect of perturbation theory in finite nuclei in order to see whether, as we suspect, perturbation theory is less justified for the surface region than for the interior.

In spite of the doubts about the validity of the method for finite nuclei, it is worth exploring simplified methods for applying it to this case.

An approach which suggests itself is to treat the attractive and the repulsive part of the two-body forces in different ways. The repulsive part is strong, and cannot be treated in perturbation theory. However, it contains mainly matrix elements relating to transitions with large momentum transfer, which lead to states outside the Fermi sea. It is there-

fore not made much less effective by the Pauli principle, so that we do not lose much in speed of convergence if we express it in terms of a t matrix defined without Pauli principle, which is much easier to calculate. As regards the attractive part, this is much weaker; and, as we have seen before, may reasonably be tackled with ordinary perturbation theory, in which case the Pauli principle takes care of itself.

This idea was used in the paper by Gomez, Walecka and Weisskopf who, however, did not examine all the more complicated correction terms which arise from the fact that the two parts of the potential have in the first step been treated in different ways. From some work now being carried out by J. Levinger, it appears that in the case treated by Gomez et al., in which the attractive potential is of a square-well shape, all these corrections are really small, but that the problem is more difficult if one works with more realistic forces of the Gammel-Thaler type since their rapid rise at smaller distances makes them less favourable for perturbation theory.

The difficulties in handling the Brueckner technique for finite nuclei make it still interesting to consider alternative ways of handling hard-core interactions, which may be less powerful, but would be easier to handle. Of these the most promising seems to be the method proposed by Jastrow.¹⁵

This starts from the variation principle, with a trial function of the form

$$\Psi = \prod_{i < j} f(r_{ij}) \Phi \quad (35)$$

where Φ is a Slater determinant and f is a function of the mutual distance of two nucleons, with the property that

$$\begin{aligned} f(r) &= 0, & r \leq a, \\ f(r) &\rightarrow 1, & r \rightarrow \infty. \end{aligned}$$

We may either choose for f a function of a reasonable form containing one or more parameters, or we may leave the form of f arbitrary and try to determine it from the variation principle.

The idea of such a trial function is very old; it was used already by Lenz to estimate the ground-state energy of a system of bosons with hard-sphere interactions. (In the case of bosons, the Slater determinant Φ has to be replaced by a symmetric function, or for uniform matter, by unity.)

It is, however, very difficult to do any calculation with such a trial function, because it is impossible to separate the variables, and success depends on finding an approximate way of dealing with it.

For example, if we consider the normalization integral, the integrand contains the factor $N f_1^2$ which, with the definition

$$f^2 = 1 - g$$

can be written as

$$\prod_{i < j} [1 - g(r_{ij})].$$

Now if the density is reasonably low, most of the g terms will be zero, since only a few of the particles will be close enough together for f to differ appreciably from unity. One is therefore tempted to expand the product, treating the g as small; but since the number of factors in which g is appreciable will always be large, this is clearly not legitimate.

This kind of problem is familiar in statistical mechanics where the "cluster" method has been developed to deal with it. In this method we define a set of functions u_1, u_2, \dots as follows:

Let

$$\begin{aligned} u_1(r) &= 1, \\ f^2(r_1) &= u_1(r_1)u_1(r_1) + u_2(r_1, r_2). \end{aligned} \tag{36}$$

This equation defines u_2 , and evidently u_2 vanishes when the two particles are so far apart that the correlation function f is practically equal to unity. Similarly

$$\begin{aligned} f^2(r_{12})f^2(r_{23})f^2(r_{31}) &= u_1(r_1)u_1(r_2)u_1(r_3) + u_1(r_1)u_2(r_1, r_2) \\ &\quad + u_1(r_2)u_2(r_1, r_3) + u_1(r_3)u_2(r_1, r_2) + u_3(r_1, r_2, r_3) \end{aligned} \tag{37}$$

gives a definition of u_3 . Again u_3 vanishes unless the particles form a "linked cluster." By this we mean a configuration of points which cannot be subdivided into smaller clusters in such a way that all the particles of one cluster are separated from all the particles of another cluster by such a distance than the correlation function f connecting them is unity.

Continuing in this way, we can express the product of all correlation functions in terms of a sum of the cluster functions u_1 to u_N . The approximation now consists in neglecting all the u except the first few.

In the boson case it is known that this method does not converge well except at low density. Jastrow showed that in the case of fermions it works at much higher densities, since the Pauli principle again helps to reduce the probability of several nucleons getting close together.

General formulae for the cluster expansion for this case were given by Iwamoto and Yamada.¹⁶ Dabrowski¹⁷ made an attempt to apply this method to a finite nucleus. There still appear to be some theoretical difficulties, since, if one leaves the form of f completely arbitrary and stops, for example, at the two-body clusters, the variation integral

has no proper minimum. The function tends to a form in which higher-order clusters would, in fact, not be negligible.

Recently, De-Shalit and Weisskopf¹⁸ have shown an interesting connection between the Brueckner and the Jastrow methods. Writing the Slater determinant Φ which occurs in both expressions in the form

$$\Phi(r_1, \dots, r_N) = \frac{1}{\sqrt{N!}} \sum_P (-1)^P U_{\alpha_1}(r_1) U_{\alpha_2}(r_2) \dots U_{\alpha_N}(r_N) \quad (38)$$

where $\alpha_1, \alpha_2, \dots, \alpha_N$ form a permutation P of the first N one-particle states and the sum is over all permutations, they show that the leading term in the Brueckner expansion for the energy is the expectation value of the Hamiltonian for the trial function

$$\Psi = \frac{1}{\sqrt{N!}} \sum_P (-1)^P \prod_{i < j} f_{\alpha_i \alpha_j}(r_i, r_j) U_{\alpha_1}(r_1) U_{\alpha_2}(r_2) \dots U_{\alpha_N}(r_N) \quad (39)$$

where the functions $f_{\alpha_i \alpha_j}(r_i, r_j)$ are the ratios between plane waves and the Bethe-Goldstone solution:

$$\Psi_{B-G}(r_i, r_j) = f_{\alpha_i \alpha_j}(r_i, r_j) U_{\alpha_i}(r_i) U_{\alpha_j}(r_j) . \quad (40)$$

This differs from the Jastrow trial function Eq. (35) in that the correlation factor in Eq. (39) is different according to the states in which the two particles are placed in the term under consideration.

This illustrates both the degree of refinement lost in the Jastrow approach in which the correlation is taken to be the same for any pair of particles, and also the reason why this approach is rather simpler to handle.

II. Nuclear Reactions and the Optical Model

Much progress has been made in the understanding of nuclear reactions by considering the incident particle as moving in an average potential well, the so-called optical potential. We shall not discuss here the methods by which one fits empirical potentials to the observed scattering cross sections and angular distributions, nor the detailed results obtained from such fits. Our purpose will be to try to understand the relation of this model to the full many-body problem.

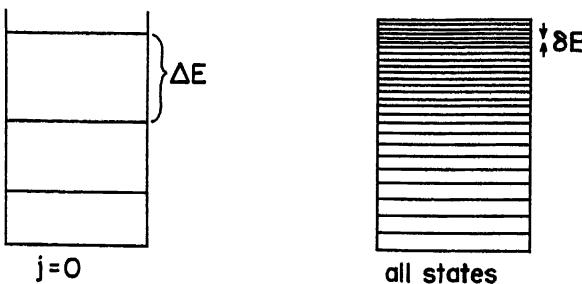
A characteristic of nucleon-nucleus collisions are the many sharp resonances at low energy (kinetic energies of the order of 1 Mev or less) more easily observed in the case of neutrons, which, at higher energies, become broader and finally merge completely.

Superimposed in this fine structure, explained by Niels Bohr as

resonance levels of the compound nucleus, there is a modulation, the so-called "giant resonances." These are regions in which the compound resonances are particularly strong.

As a guide to the situation with which we are here concerned, it is useful to start by considering a model in which the incident nucleon has no interaction with the nucleons in the target nucleus, and then to consider the effect of this interaction.

In the non-interacting model the energy of any level will be the sum of the energy ϵ_j of the j -th state of the target and the energy E_m of a one-particle resonance of the extra nucleon in whatever field of force we take it to be moving. The spectrum of all these levels will, at the energies with which we are concerned, be very dense. We may, however, divide it into the states $j = 0$, i. e., with the target nucleus in the ground state, which will be of special importance for the process, and the rest. The $j = 0$ states are fairly widely spaced, whereas the rest is dense.



We distinguish the spacing ΔE , of the $j = 0$ levels which will be many Mev, from the spacing of all compound levels, δE , which may be perhaps 100 ev. As long as there is no interaction, the target nucleus will remain in the state $j = 0$, and the scattering will go entirely through the single-particle resonances shown in the left-hand diagram. Their width is the single-particle resonance width, which depends on the nature of the field of force.

Now if we add the interaction, the results of our previous discussion of the shell model might suggest that we should treat this as a small perturbation. It is, however, obvious that perturbation theory in the usual sense would fail completely. The criterion for its validity is again that the ratio of the interaction to the distances between unperturbed energy levels be small (see Eq. (17)), and here we have to count all levels of the system; so we must compare the interaction W with δE . Near the ground state of the system, with which we are concerned in the shell model, δE is the same as ΔE . However, for a system of target plus extra nucleon, we are above the ground state by the binding energy of one nucleon, i. e., by about 6-8 Mev, and δE is so small that there is no hope

at all of justifying perturbation theory.

Indeed the eigenstates of the compound system will be mixtures of many of the uncoupled states defined above. We can see easily that in this mixture all those uncoupled states will occur with appreciable coefficients whose unperturbed energies differ from the actual energy by less than the magnitude of the interaction W .

Now since, in the absence of interaction, the collision process is described entirely by the $j = 0$ states, a compound resonance will occur only to the extent to which its expansion into uncoupled states contains a $j = 0$ state. In other words, we expect the compound resonances to be strong in regions of width W around the single-particle resonances. Thus these giant resonances will be distinct as long as W is less than the spacing of the single-particle resonances, or

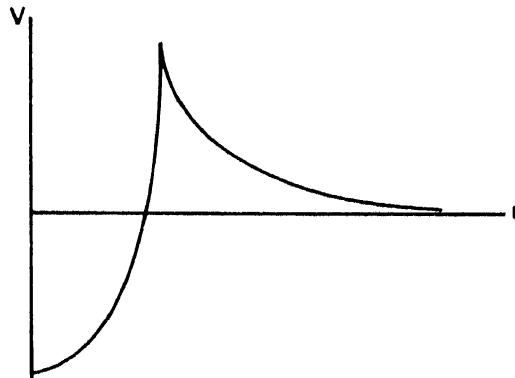
$$W < \Delta E .$$

This condition may easily be satisfied in many cases, whereas the condition $W < \delta E$, which would permit perturbation theory, will never be.

We can look at this problem from the point of view of time-dependent perturbation theory. In this case we have at time $t = 0$ the asymptotic form with the nucleus in the ground state and the particle in one of the levels of the potential well. Because of the interaction between the particles, the states will become mixed, and therefore the amount of the original state will decrease. This is the reason we have to introduce the complex potential, in order to account for this absorption.

We shall follow a procedure developed by Kapur and Peierls.¹⁹ This method is equivalent to the better-known method by Wigner and Eisenbud, but for our present purpose turns out to be more convenient because it involves a linear relation between the scattering amplitude and a sum of resonance terms.

We will begin our discussion with the problem of a particle confined by a potential barrier. This is the familiar problem of α -decay.



One way to proceed would be to assume that at some time the particle was definitely in the well. However, there is no unique prescription for doing this. Furthermore, for an actual nucleus, we do not suppose that we have actually made a measurement to determine whether or not the alpha particle is in the nucleus, or already on the way out. An alternative procedure is to suppose that the nucleus has always been emitting α particles, and has an exponentially diminishing strength. That is, we can look for solutions of the form:

$$\Psi = u(x) e^{-iWt/\hbar}$$

with

$$W = E - i\Gamma/2$$

then

$$|\Psi|^2 = |u(x)|^2 e^{-\Gamma t/\hbar}.$$

The wave equation is:

$$\frac{\hbar^2}{2m} \nabla^2 u + (W - V)u = 0.$$

If we put $W \rightarrow W^*$ then u^* is another solution of the equation. The physically meaningful solution is selected by the boundary condition that at infinity we have only outgoing waves. That is:

$$ru \rightarrow e^{+ikr} \quad \text{as} \quad r \rightarrow \infty.$$

With this boundary condition the answer is uniquely determined. Sometimes this method was claimed to be unsatisfactory for the following reason. As

$$r \rightarrow \infty, \quad V(r) \rightarrow 0$$

and we are left with:

$$\frac{\hbar^2}{2m} k^2 = W.$$

Therefore, k must be complex. Furthermore, the imaginary part of k is negative. This means that the wave function increases as $\exp[i\text{Im } k]r$. This is no difficulty, however. It merely results from the fact that with our idealization, the source was much stronger in the

distant past; and we see at large distance the numerous α particles emitted a long time ago.

We shall digress for a moment to show an application of this procedure to scattering in the neighborhood of a resonance. This discussion is applicable only in the case where the width Γ of the level is much less than the distance d between resonances. This is normally the case for neutron reactions of not too high energies. Now we expect to find appreciable scattering only when $|E - E_0| < \Gamma$ where E is the bombarding energy, and E_0 is the energy of the resonance level. Since $\Gamma \ll d$, we have only one level in this range, and therefore we are dealing with a unique quantum state of the compound nucleus. The possibility of exciting some other state is negligible. Then we can assume that all the compound nuclei which are formed by these collisions are identical. This has two consequences. First, the decay probability cannot depend upon the time for which the states have been sitting there. Therefore, the decay must be purely exponential, of the form used for the previous problem.

Furthermore, since the compound states are identical, and therefore indistinguishable, the probabilities for the separate modes of decay must be independent of the manner in which the compound state was formed.

If we denote by Γ_a the particle width for decay into channel a, say, then the transition probability is given by:

$$\Gamma_a / \hbar = \lambda_a .$$

Also, Γ_a / Γ must be a constant independent of the process of formation. Then if we denote the system with the incident particle as a, we can write the cross section for scattering from channel a to some channel b, say, by:

$$\sigma_{ab} = \sigma_a^c \frac{\Gamma_b}{\Gamma} \quad (41)$$

where σ_a^c is the cross section for the formation of the compound nucleus. Therefore, it only remains for us to calculate σ_a^c . Because the state of the compound nucleus is an exponentially decaying state, we know the cross section must have the form

$$\sigma_a^c = \left| \frac{A}{(E - E_0) + i\Gamma/2} \right|^2 \quad \text{where } A \text{ is some constant.} \quad (42)$$

Now this constant A may easily be determined by the principle of detailed balancing. We consider the compound nuclei in equilibrium with the bombarding particle and the target nuclei, in some suitable enclosure. Then, in such an equilibrium situation, the number of compound nuclei formed must just equal the number which decay.

We must here not fix the energy E too closely, for in doing so we may introduce uncertainties in the time which may be greater than the decay time of the nuclei. Therefore we take an energy interval ΔE such that $\Delta E \gg \Gamma$. However, we still suppose that $\Delta E \ll d$. Now the number of particles in the given energy range is given by:

$$\frac{V}{(2\pi\hbar)^3} (4\pi p^2 dp) = \frac{V}{(2\pi\hbar)^3} (4\pi p^2) \frac{\Delta E}{\Gamma} .$$

Therefore the number of compound nuclei formed per second is just the flux density times the cross section averaged over the interval ΔE . Therefore we have:

$$\frac{4\pi p^2 \Delta E}{(2\pi\hbar)^3} \frac{\int_{\Delta E} \sigma_a^c dE}{\Delta E} = \frac{\Gamma_a}{\hbar} .$$

Since we assume $\Delta E \gg \Gamma$, we can extend the limits of integration of ΔE to $\pm\infty$ without changing anything. Then we have:

$$\int_{-\infty}^{+\infty} \sigma_a^c dE = \Gamma_a \frac{\hbar^2}{p^2} 2\pi^2 \quad (43)$$

or we can write, using Eq. (42),

$$\int_{-\infty}^{+\infty} \frac{A^2 dE}{(E-E_0)^2 + \Gamma^2/4} = A^2 \frac{2\pi}{\Gamma} .$$

Therefore,

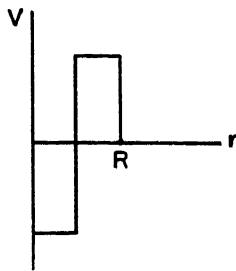
$$A^2 = \pi \Gamma \hbar^2 \Gamma_a / p^2 \quad (44)$$

and we find, using Eq. (41),

$$\sigma_{ab} = \pi \lambda^2 \frac{\Gamma_a \Gamma_b}{(E-E_0)^2 + \Gamma^2/4} .$$

This is the simplest form of the Breit-Wigner one-level formula, in which we have neglected spin completely. We only want to emphasize how few assumptions, and how little mathematics is needed to obtain this result.

As a first step towards generalizing this procedure to take care of systems with many resonances, we shall first discuss a system consisting of one particle, in an S state. Later, we will generalize this procedure to take into account the many decay channels which are available to nuclei of more than one particle. We consider one particle in a well shaped somewhat as follows:



The Schrödinger equation is:

$$\frac{\hbar^2}{2m} \nabla^2 u_n + (W_n - V) u_n = 0 \quad (45)$$

where

$$u = 0 \quad \text{at} \quad r = 0$$

furthermore, for

$$r > R, \quad V = 0$$

and

$$k_n = \sqrt{\frac{2m}{\hbar^2} W_n} \quad .$$

In the region $r > R$ we assume only outgoing waves, so

$$u \sim e^{+ikr} \quad .$$

The boundary conditions can be written as:

$$\frac{du_n}{dr} - ik_n u_n = 0 \quad \text{at} \quad r = R \quad .$$

Now we can restrict our discussion entirely to the region $r < R$. The set of functions satisfying these boundary conditions are probably a complete set, but they are not orthogonal over the region R because they all satisfy different boundary conditions. However, the dependence on n is not very great, as we shall see in detail later, and it is convenient to replace these boundary conditions by the following ones:

$$\frac{du_n}{dr} - iK u_n = 0 \quad \text{at} \quad r = R. \quad (46)$$

Here K is the wave vector for the incident particle. Now these functions are orthogonal in the sense that:

$$\int_0^R u_n u_l dr = 0 \quad \text{for} \quad n \neq l.$$

We choose units with

$$\frac{\hbar^2}{2m} = 1$$

and write

$$\frac{d^2 u_n}{dr^2} + (W_n - V) u_n = 0$$

and

$$\frac{d^2 u_l}{dr^2} + (W_l - V) u_l = 0;$$

then multiplying the first equation by u_l and the second by u_n and subtracting, we obtain after integrating over the interval 0 to R :

$$\int_0^R \left[u_l \frac{d^2 u_n}{dr^2} - u_n \frac{d^2 u_l}{dr^2} \right] dr + (W_n - W_l) \int_0^R u_n u_l dr = 0.$$

Integrating the first term by parts, and using the boundary conditions, we get:

$$\left| u_l \frac{du_n}{dr} - u_n \frac{du_l}{dr} \right|_0^R = 0;$$

therefore

$$(W_n - W_l) \int_0^R u_n u_l dr = 0 .$$

If $W_n \neq W_l$, then we have orthogonality.

Completeness is harder to prove, but the functions do form a complete set, subject to some requirements on the potential. The functions are complete only in the sense that:

$$F(x) = \sum_n c_n u_n(x)$$

where F is an arbitrary function that satisfies the boundary condition Eq. (46). If F has this form we can write:

$$c_n = \frac{\int_0^R u_n(r) F(r) dr}{\int_0^R u_n^2 dr} \quad (47)$$

We must be careful that

$$\int_0^R u_n^2 dr$$

does not vanish. This is possible since u_n is complex, but this exceptional case will be discussed later. Otherwise we may assume that the u_n are normalized in the sense that

$$\int_0^R u_n^2 dr = 1 ,$$

then:

$$c_n = \int_0^R u_n(r) F(r) dr . \quad (48)$$

If we take the complex conjugate of the Schrödinger equation, we have:

$$\frac{d^2 u_i^*}{dr^2} + (W_i^* - V) u_i^* = 0$$

$$\frac{d^2 u_n}{dr^2} + (W_n - V) u_n = 0 .$$

Now multiply by u_n and u_i^* and integrate. We get

$$- \left(u_i^* \frac{du_n}{dr} - \frac{du_i^*}{dr} u_n \right) \Big|_0^R + (W_n - W_i^*) \int_0^R u_n u_i^* dr = 0 .$$

Now the first term does not vanish. We get

$$- 2iK(u_i^* u_n)_R + (W_n - W_i^*) \int_0^R u_n u_i^* dr = 0 .$$

Consider the case with $n = l$. Then:

$$2iK(u_i^* u_n)_R = 2i|\text{Im } W_n| \int_0^R u_n u_i^* dr ;$$

therefore:

$$\frac{\Gamma_n}{\hbar} = \frac{\hbar K}{m} \frac{|u_n(R)|^2}{\int_0^R |u_n(r)|^2 dr} . \quad (49)$$

This equation has a very simple interpretation. It just says that the escape probability is equal to the velocity times the probability for finding the particle on the surface, divided by the probability for finding the particle somewhere in the interior.

Now let us generalize somewhat to take into account the case with $l \neq 0$ and for Coulomb wave function. In this case we must replace

$$e^{+ikr}$$

by

$$\Psi^+(k) .$$

The plus sign indicates that we choose the outgoing Coulomb wave. The boundary condition then becomes:

$$\frac{du}{dr} - f_+ u = 0 \quad \text{at} \quad r = R$$

where

$$f_+ = \left(\frac{1}{\Psi^+} \frac{d\Psi^+}{dr} \right)_R .$$

Now let us return to the exceptional case in which

$$\int_0^R u_n^2 dr = 0.$$

When this happens our functions no longer form a complete set. Consider the Schrödinger equation

$$\frac{d^2u}{dr^2} + (W - V(r))u = 0 .$$

(For states with $\ell \neq 0$ we can consider the centrifugal term as included in the $V(r)$.) Now the set of values W , which in general may be complex, will depend upon f_+ . However, we may also consider f_+ as a function of W , and it is then single valued and analytic. Consider the following:

$$\frac{d^2\bar{u}}{dr^2} + (\bar{W} - V)\bar{u} = 0$$

$$\frac{d^2u}{dr^2} + (W - V)u = 0 .$$

Here we consider \bar{W} as slightly different from W . If we multiply by u and \bar{u} , and integrate, we obtain, upon subtraction and integration by parts:

$$\left(\bar{u} \frac{du}{dr} - u \frac{d\bar{u}}{dr} \right) + (W - \bar{W}) \int_0^R u \bar{u} dr = 0.$$

Now the equation becomes:

$$(f_+ - \bar{f}_+) (u \bar{u})_R + (W - \bar{W}) \int_0^R u \bar{u} dr = 0.$$

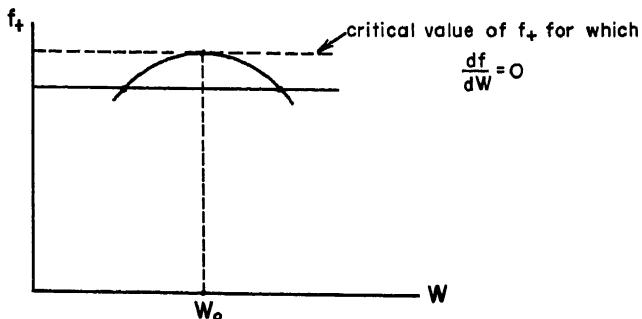
If we now go to the limit where $\bar{W} \rightarrow W$ we may write

$$\frac{df_+}{dW} = - \frac{1}{(u^2)_R} \int_0^R u^2 dr.$$

Now $u^2(R)$ will never vanish, since if it did, $u=0$ would be the solution to our equations. Therefore, the only time the integral vanishes is when

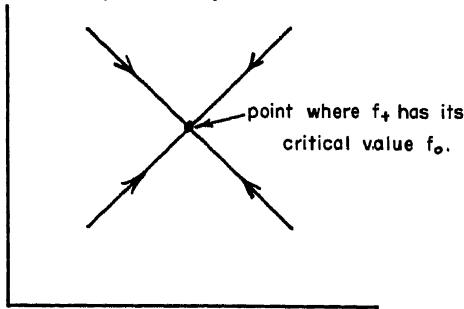
$$\frac{df_+}{dW} = 0.$$

Since both f_+ and W are complex, we cannot plot f_+ against W . However, we may picture it symbolically as follows:



Now for f_+ less than the critical value, we will have two values of W . The behavior of W for f_+ greater than the critical value may be seen by following the points in the complex W plane, for f_+ following some path in the complex plane through the exceptional point.

Complex W plane



This will be true at least when

$$\frac{df_+}{dW} = 0$$

but

$$\frac{df_+}{dW} \neq 0 .$$

In the neighborhood of the point $f_+ = f_0$ we can write:

$$f_+ = f_0 + \alpha(W - W_0)^2.$$

Now it is clear how we may obtain a complete set of functions. Since the equations are linear,

$$(u_{W_1} + u_{W_2})/2$$

is also a solution, and furthermore, as we approach f_0 we just get the solution W_0 . Since the set

$$(u_{W_1} + u_{W_2})/2$$

and

$$(u_{W_1} - u_{W_2})/2$$

form an orthonormal set, we lose the solution

$$(u_{W_1} - u_{W_2})/2$$

as $W \rightarrow W_0$, and have to add in du/df_+ , although this will not satisfy the Schrödinger equation. Another method would be to consider the problem with f_+ slightly different from f_0 and then take the solutions in the limit as $f_+ \rightarrow f_0$. Since it is unlikely that we shall run into such an exceptional case in practice, we shall not pursue this exceptional case further.

A more important generalization of our equations takes into account the many-body problem. What we have here is a wave function:

$$\Psi = \Psi(r_1, \dots, r_N).$$

Let us consider this wave function for the case where any one of the r_i 's, r_i say, becomes large. Then we have $r_i > R$. Now we can write

$$\Psi = \Psi(r_i, \Omega_1, r_2, \dots, r_N)$$

or

$$\Psi = \sum_j Y_{lm}(\Omega_1) X_j(r_2, \dots, r_N) u_{lmj}(r_i). \quad (50)$$

If

$$r_i > R, \quad u_{lmj}$$

must satisfy the one-particle equation. Therefore the boundary conditions can be written in terms of:

$$\left(\frac{1}{u_{lmj}} \frac{du_{lmj}}{dr} \right)_{r_i=R} = f_{+l}(k_j) \quad (51)$$

The subscript l on f_+ will only indicate whether the particle is a proton or a neutron. The j dependence of f_+ arises from the fact that the energy of the residual state will depend upon the energy of the outgoing particle.

We shall speak of a channel as being specified by the nature and angular momentum of the outgoing particle and the state of the residual nucleus. Then l, m and j specify the channel. We shall not discuss spin in what follows.

Now let us treat the scattering problem. We shall again first discuss the simple case of the single particle in a potential well and restrict ourselves to S-wave neutrons. Then for $r > R$:

$$\Psi = I \sin kr + S e^{ikr}$$

where I is the amplitude of the incoming wave, and S the amplitude of

the scattered wave. Now for $r < R$ we can write:

$$\Psi = \sum_n c_n u_n + \text{corrections for the boundary conditions.}$$

These added correction terms are present because all the u_n satisfy the homogeneous boundary condition. The wave for $r > R$ cannot possibly satisfy this, since it contains both ingoing and outgoing waves. Because the wave functions must be matched at the boundary, we must include extra terms in the expansion of Ψ for $r < R$. This was the method used in the paper by Kapur and Peierls. However, it will be convenient at this point to take a slightly more general view.

We write for $r < R$,

$$\Psi(r) = \hat{\Psi}(r) + \Psi_i(r) \quad (52)$$

where $\hat{\Psi}$ is a solution for the optical potential, for which we assume that we can solve the Schroedinger equation,

$$\frac{d^2 \hat{\Psi}}{dr^2} + (k^2 - \hat{V}) \hat{\Psi} = 0$$

and for $r > R$, we have

$$\hat{\Psi} = I \sin kr + S e^{ikr}.$$

Now Ψ , contains only outgoing waves, and can be written:

$$\Psi_i = \sum_n c_n u_n \quad \text{for } r < R;$$

for $r > R$ we write:

$$\Psi_i = S_i e^{ikr}. \quad (52)$$

If we take the special case where $\hat{V} = \infty$ for $r < R$, we obtain:

$$\hat{\Psi} = 0 \quad \text{for } r < R.$$

Then $\Psi = \Psi_i$ for $r < R$. Then for this case we obtain the old way of expanding Ψ in the interior. Now let us insert the solution

$$\Psi = \hat{\Psi} + \sum_n c_n u_n$$

into the Schroedinger equation. We obtain:

$$\frac{d^2\hat{\Psi}}{dr^2} + (k^2 - V)\hat{\Psi} + \sum_n c_n \left[\frac{d^2u_n}{dr^2} + (k^2 - V)u_n \right] = 0 .$$

We can find c_n by the orthonormality relations for the u 's.

$$c_n = \frac{\int_0^R u_n(x)(V - V)\hat{\Psi}(x)dx}{k^2 - W_n} .$$

Hence, by continuity at R with Eq. (52):

$$S_1 = e^{-ikR} \hat{\Psi}(R)$$

or

$$S_1 = e^{-ikR} \sum_n \frac{\left[\int_0^R u_n(r)(V - V)\hat{\Psi}(r)dr \right]}{k^2 - W_n} u_n(R) . \quad (53)$$

This is now a formally exact expression for the scattering amplitude S_1 . Similarly, in the general case:

$$S_{ab} = \hat{S}_a \delta_{ab} + \sum_n \frac{\langle a | V - \hat{V} | n \rangle \langle u_n(R, b) \rangle}{(E - W_n) \phi_b^+} \quad (54)$$

where we are scattering from channel a to channel b. Here

$$\langle a | V - \hat{V} | n \rangle = \int \hat{\phi}_a(r_a) Y_{l_a m_a}(\Omega_a) X_a(\xi_a) [V - \hat{V}] u_n d\tau$$

where

$$\xi_a = (r_1, \dots, r_{a-1}, r_{a+1}, \dots, r_N) .$$

X_a is the wave function of the residual nucleus for channel a.

$$\langle u_n(R, b) \rangle = \int u_n(r_1, \dots, R \Omega_b, \dots, r_N) Y_{l_b m_b} X_j(\xi_b) d\xi_b d\Omega_b . \quad (55)$$

ϕ_b^+ is the amplitude of the outgoing wave in channel b, i. e.,

$$\frac{\hbar^2}{2m} \nabla^2 \phi_b^+ + (E_b - V_{\text{coul}}) \phi_b^+ = 0.$$

These equations are derived in exactly the same manner as we did for the single particle case, the complications arising from the increased number of variables. These formulas may be found in a paper by G. E. Brown and De Dominicis.²⁰ A similar result is also used by J. Bowcock.²¹

We now have the problem of evaluating this expression. We shall try to minimize the effect of the last term by choosing \hat{V} in such a way that \hat{S} gives the average scattering amplitude. This will tend to make the sum as insensitive as possible to the high-energy compound resonance levels.

It is convenient to put Eq. (54) in a somewhat different form, since we know, from detailed balancing, that there is a close relation between S_{ab} and S_{ba} . This symmetry is not apparent in Eq. (54) for S_{ab} . We can write this expression in another form which will make this symmetry more apparent. To begin with we derive the following identity. Let us abbreviate:

$$\Psi_a = \hat{\Phi}_a Y_{l_a m_a}(\Omega) X_a(\xi_a).$$

Now:

$$(E - \hat{H}) \Psi = 0$$

and

$$(W_n - H) u_n = 0.$$

Multiplying by u_n and Ψ and integrating, we get upon subtraction:

$$\begin{aligned} & \int u_n (V - \hat{V}) \Psi_a d\tau + (E - W_n) \int u_n \Psi_a d\tau + \\ & + \frac{\hbar^2}{2m} \sum_b \left(u_n \frac{\partial \Psi}{\partial r_b} - \Psi \frac{\partial u_n}{\partial r_b} \right)_{R,b} = 0. \end{aligned} \quad (56)$$

The last term arises from the non-vanishing terms when we do the integration by parts over the kinetic energy terms. Our notation here is slightly symbolic. We take the function on the surface in configuration space which corresponds to channel b, average out the nuclear variables, and average the appropriate spherical harmonic over the surface. The

m which appears here is the reduced mass of the emitted fragment and the residual nucleus, and in most cases is practically equal to the nucleon mass.

The last term can be written as:

$$u_n(R, b) \left(\frac{\partial \hat{\Psi}}{\partial r_b} - f_{+b} \hat{\Psi} \right).$$

Now this term vanishes when $\hat{\Psi}$ satisfies the homogeneous boundary conditions. This is true in fact for all channels except channel a . We can therefore write the last term as:

$$\frac{\hbar^2}{2m} u_n(R, a) \left(\frac{\partial \hat{\Psi}}{\partial r_a} - f_{+a} \hat{\Psi} \right).$$

Outside of R we can write:

$$\hat{\Psi} = I(\phi^+ - \phi^-) + \hat{S} \phi^+$$

and from continuity,

$$\left(\frac{\partial \hat{\phi}}{\partial r} - f_+ \hat{\phi} \right)_R = - I(f_- - f_+) \phi^-(R).$$

The ϕ^+ terms all vanish because they satisfy the homogeneous boundary condition. We can simplify this further by making use of the fact that ϕ^+ and ϕ^- are both solutions of the Schrödinger equation. Therefore they satisfy the Wronskian identity:

$$\phi^- \frac{\partial \phi^+}{\partial r} - \phi^+ \frac{\partial \phi^-}{\partial r} = \text{const.}$$

We can arrange this constant to be unity by proper choice of the arbitrary factor in ϕ^- . This gives us

$$(f_+ - f_-) \phi^+(R) \phi^-(R) = 1.$$

Now we can substitute this into the identity of Eq. (56) and obtain:

$$-\frac{\hbar^2}{2m} u_n(R, a) \frac{I}{\phi^+_a(R)} + \int u_n(V - \hat{V}) \hat{\Psi}_a d\tau + (E - W_n) \int u_n \hat{\Psi}_a d\tau = 0. \quad (57)$$

We can make use of this identity in two ways. First, we may use it to eliminate the matrix element of $(V - \hat{V})$ in our expression for S_{ab} . We get:

$$S_{ab} = \hat{S}_a \delta_{ab} - \frac{1}{\phi_b^+} \sum_n \langle u_n \hat{\Psi}_a u_n(R, b) \rangle d\tau + \frac{\hbar^2}{2m} \frac{I_a}{\phi_a^+ \phi_b^+} \sum_n \frac{\langle u_n(R, a) \rangle \langle u_n(R, b) \rangle}{E - W_n}.$$

The summation in the second term may be done by using the closure relation, and we get a delta function over the boundary of channel b. Then we get:

$$S_{ab} = \hat{S}_a \delta_{ab} - \frac{\langle \hat{\Psi}_a(R, b) \rangle}{\phi_b^+} + \frac{\hbar^2}{2m} \frac{I_a}{\phi_a^+ \phi_b^+} \sum_n \frac{\langle u_n(R, a) \rangle \langle u_n(R, b) \rangle}{E - W_n}. \quad (58)$$

This displays some of the symmetry between a and b in the scattering amplitude. The last term is what one would expect from a generalization of the Breit-Wigner formula for more than one resonance. The ϕ^+ 's are related to the partial widths of the resonance. But Eq. (58) is not yet completely symmetric.

We can use our identity in another way. One may eliminate $u_n(R, b)$ from the equation for the scattering amplitude. One finds:

$$\begin{aligned} S_{ab} = & \hat{S}_a \delta_{ab} - \frac{2m}{\hbar^2} \frac{1}{I_b} \langle b | V - \hat{V}_a | a \rangle \\ & - \frac{2m}{\hbar^2} \sum_n \frac{\langle b | V - \hat{V}_b | n \rangle \chi_n | V - \hat{V}_a | a \rangle}{E - W_n} \end{aligned} \quad (59)$$

This is just the perturbation theory result with a term added to give the resonances.

This result is exact, and valid for any choice of the "well potential" \hat{V} . It is not yet, however, of great practical use, since we can never calculate all terms in the resonance sum, and must therefore look for a choice of \hat{V} which will make the contribution from this sum unimportant.

This can be done by connecting the compound states with the states of the target nucleus and the extra nucleon, using a method given in the paper by Lane, Thomas and Wigner.²²

The functions

$$\Psi_{mj} = \chi_j(\xi_a) \hat{\phi}_n(r_a) Y_{lm}(\Omega_a) \quad (60)$$

where $\hat{\phi}_n$ is an eigenfunction in the well potential

$$(\epsilon_m - T - \hat{V}) \hat{\phi}_m = 0$$

with the boundary condition

$$\left(\frac{\partial \hat{\phi}_m}{\partial r} - f_+ \hat{\phi}_m \right)_R = 0$$

form a complete set, so that the compound states u_n can be expanded

$$u_n = \sum_{m,j} a_{mj}^n \Psi_{mj} . \quad (61)$$

If $j = 0$ denotes the ground state, we shall be interested particularly in the coefficient a_{m0}^n . It will turn out that this is large only if $W_n \sim \epsilon_{m0}$.

Inserting the expansion Eq. (61) into the Schrödinger equation for u_n we obtain easily

$$(W_n - \epsilon_{mj}) a_{mj}^n = \sum_{m'j'} \langle m'j' | V - \hat{V} | mj \rangle a_{m'j'}^n . \quad (62)$$

From the completeness relations for the u_n we obtain

$$\sum_n a_{mj}^n a_{m'j'}^n = \delta_{mm'} \delta_{jj'} \quad (63)$$

and in particular

$$\sum_n (a_{mj}^n)^2 = 1.$$

Multiplying Eq. (62) by a_{mj}^n and summing over n :

$$\bar{W} \equiv \sum_n W_n (a_{mj}^n)^2 = \epsilon_{mj} + \langle mj | V - \hat{V} | mj \rangle . \quad (64)$$

Similarly, one can show that

$$\overline{(W_n - \bar{W})^2} = \langle mj | (V - \hat{V})^2 | mj \rangle - \langle mj | V - \hat{V} | mj \rangle^2 . \quad (65)$$

The results Eqs. (64) and (65) show that the uncoupled state m, j is contained mostly in those compound states whose energy is close to the uncoupled energy, ϵ_{mj} , shifted by the average value of the coupling term $V - \hat{V}$ and that this contribution is limited to a range of compound energies which depends on the fluctuations of this coupling term, but is independent of the density of compound states.

This expansion in uncoupled states also shows us the way to choose \hat{V} . We would like the optical scattering S to be the dominant part. It cannot, of course, reproduce the fine structure of the compound

resonances, but can represent the average scattering amplitude; and in the region of higher energies where the compound resonances overlap, it may approximate to the actual amplitude. In any event, since the distant terms in the dispersion sum produce only a slowly varying background, we want this absorbed into the optical amplitude so that the sum converges rapidly.

We start from Eq. (54) for elastic scattering, $b = a$. Using the expansion Eq. (61), we find easily for the dispersion sum:

$$\frac{1}{\phi_a^+} \sum_n \sum_{m'_j, m} \frac{\hat{\phi}_m(R) \langle j, m | V - \hat{V} | 0, \alpha \rangle a_m^n a_{m'}^n}{E - W_n}$$

At this point we have taken no account of the identity of the incident particle with the target nucleons, which requires an antisymmetrized wave function. The expansion Eq. (61) is, of course, legitimate in any case, but the identity of the particles means that we may reach the channel a also by taking one of the nucleons contained in the ξ_a of Eq. (60) to the nuclear surface and forming the target ground state from the remaining nucleons plus r_a . Our formulae are therefore applicable directly only to a case in which the incident particle is distinguishable from the others, but it is likely that an incorporation of exchange effects would not seriously alter the position.

We now remember the fact that a_m^n is appreciable only when W_n is near ϵ_{m0} . This suggests approximating W_n in the denominator by ϵ_{m0} . If the actual energy, E , is close to ϵ_{m0} , i. e., within the m -th giant resonance, this is not a good approximation, but it is certainly good for the distant resonances. With this approximation, the denominator is independent of n ; and we can do the summation over n , using the completeness relation Eq. (63). The result is

$$\frac{1}{\phi_a^+} \sum_m \frac{\hat{\phi}_m(R) \langle m, 0 | V - \hat{V} | 0, \alpha \rangle}{E - \epsilon_{m0}} \quad (66)$$

To this approximation we may easily make the sum vanish by taking

$$\hat{V}(r) = \int \chi^*(\xi) V(r, \xi) \chi_0(\xi) d\xi \quad (67)$$

which will make every term in the sum Eq. (65) vanish. This is just the Hartree potential for the extra particle, with the target nucleus in the ground state.

The optical potential Eq. (67) would be real and have no absorption. This is not surprising, since the imaginary part arises just from the resonances in the neighborhood of E , which we have not yet handled correctly.

One might here be worried that if we add an imaginary part to V this might destroy the cancellation of the distant terms we have just achieved. However, the imaginary part of the potential will influence only the width of the giant resonances and not their strength. The contribution to the sum from the distant regions comes from their wings, which are insensitive to the width.

The result Eq. (65), leading to the Hartree potential Eq. (67) was already given in the paper by Bowcock. One might think that it could be improved by correcting for the error in the denominator:

$$\frac{1}{E - W_n} = \frac{1}{E - \epsilon_{om} + (\epsilon_{om} - W_n)} = \frac{1}{E - \epsilon_{om}} - \frac{\epsilon_{om} - W_n}{(E - \epsilon_{om})^2} + \dots$$

In this series we are now concerned with positive powers of W_n , which can be evaluated in the same way as was used to derive Eqs. (64) and (65). However, the expansion does not converge when $|E - \epsilon_{om}| < |\epsilon_{om} - W_n|$. This will be of importance when the energy E lies within the m -th giant resonance. This expansion may therefore serve to improve the treatment of the distant resonances, but not handle the close ones, and thus obtain a realistic estimate of the imaginary part of the optical potential.

A more powerful approach starts, most conveniently from the form Eq. (59) for the elastic scattering. We require that the scattering be, on the average, equal to the first term, the optical scattering, and hence that the other two terms cancel on the average. It was first suggested by C. Bloch²³ that it is legitimate to treat the compound states n occurring in the sum in Eq. (59) in perturbation theory if the expression is averaged over a suitable energy interval. If this average is taken with uniform weight over a finite interval, one gets into mathematical complications from end effects. A device for avoiding such complications is used in a forthcoming paper by Brown, De Dominicis and Langer. We define the average amplitude at energy E as

$$\bar{S} = \int Q(E-E') S(E') dE'$$

and choose as the weight factor

$$Q(E-E') = \frac{B}{\pi} \frac{1}{(E-E_0)^2 + B^2} .$$

Then the corresponding average of the last term in Eq. (59) is simply obtained by replacing in the denominator $E - W_n$ by $E - W_n + iB$.

It is then evident that for sufficiently large B the denominator will never be small, and that therefore the expression is amenable to perturbation treatment. However, it is important to consider how large B has to be to make this possible.

Since, in a perturbation expansion, the energy denominators will be compared with the coupling term $V - \bar{V}$, it certainly suffices to make B larger than the magnitude of this coupling. However, this is just the magnitude of the widths of the giant resonances, and it looks therefore as if we should have to average over an interval larger than this. If the optical model could claim to be correct only for such averages, it could not be used to discuss the shape or width of the giant resonances, though it might still be used to find their position and to put an upper limit on their width. It will be seen, however, that this argument overestimates the required magnitude of B .

Our condition is now

$$\langle 0\alpha | V - \bar{V} | 0\alpha \rangle - \sum_n \frac{\langle 0\alpha | V - \bar{V} | n \rangle \langle n | V - \bar{V} | 0\alpha \rangle}{W_n - E - iB} = 0. \quad (68)$$

Let

$$\hat{V} = \nabla + \omega$$

where \bar{V} is the Hartree potential Eq. (67), and ω contains the imaginary part. (In fact, ω is almost purely imaginary.) Then the condition for ω becomes

$$\langle 0\alpha | \omega | 0\alpha \rangle = \sum_n \frac{\langle 0\alpha | V - \nabla - \omega | n \rangle \langle n | V - \nabla - \omega | 0\alpha \rangle}{W_n - E - iB}$$

which may be written in operator form as

$$\langle 0\alpha | \omega | 0\alpha \rangle = \langle 0\alpha | (V - \nabla - \omega) \frac{1}{H - E - iB} (V - \nabla - \omega) | 0\alpha \rangle. \quad (69)$$

Now Brown, De Dominicis and Langer show that this is solved by

$$\langle \alpha | \omega | \alpha \rangle = \langle 0\alpha | (V - \nabla) \frac{1}{H - \Lambda_0(V - \nabla) - E - iB} (V - \nabla) | 0\alpha \rangle \quad (70)$$

where Λ_0 is the projection operator $O^\dagger O$, i. e., picks out the component with the target nucleus in its ground state.

Now we may again try to apply perturbation theory, i. e., replace the Hamiltonian H in Eq. (70) by the uncoupled Hamiltonian, and neglect the term with $V - \bar{V}$ in the denominator. This gives

$$\langle n | \omega | m \rangle = \sum_{j'm'} \frac{\langle on | V - \nabla | jm' \rangle \langle jm' | V - \nabla | om \rangle}{\epsilon_{jm} - E - iB}. \quad (71)$$

The question is now how large must B be chosen so as to make the terms neglected in Eq. (71) negligible. The neglected terms will contain non-diagonal elements of $V - \bar{V}$ linking the state j' , m' with other states. Here the main danger arises when the state j' , m' has an uncoupled energy almost equal to E , and the transition is also to another state j'' , m'' of nearly the same energy. Otherwise, we have appreciable energy denominators independently of B . We must therefore consider real, energy-conserving transitions in which the extra particle exchanges energy with the nucleus.

But, starting from the initial single-particle resonance m , the extra particle must have gone to a lower state m' . It could not have gone to a higher state, since then the energy could not be conserved, as the target nucleus, starting from the ground state, cannot lose energy. From the state m' we could go back to m , 0, but the statistical weight of this transition is very small. Otherwise the extra particle must lose still more energy to the target.

We see, therefore, that the transitions neglected in Eq. (71) are transitions in which the incident nucleon after dropping into a lower level, loses still more energy. Hence the width with which B must be compared is not that of the giant resonance we are studying, but that for the extra particle at much lower energy. Since a particle of lower energy is much less effective in exciting the nucleus, this width is much less; and therefore B may well be less than the width of the giant resonance, and our averaging need not wash out its structure.

For this argument it is essential that the spacing of the single-particle levels is appreciable. To illustrate this point assume that we happen to have for zero kinetic energy, an S wave resonance with radial quantum number $n = 2$. The energies are, for a square well, proportional to $(n + 1/2)^2$, measured from the bottom of the well. Hence the resonance for $n = 3$ is $49/25$ times the well depth, i. e., about double. For a depth of 50 Mev, the next higher resonance therefore occurs at about 50 Mev kinetic energy.

The eigenvalues belonging to other partial waves will, in general, be different, but over a wide range all even states will lie close together, and similarly, all odd states. This is due to the fact that, in a flat-bottomed well, the wave function in the interior is given by a spherical Bessel function, whose asymptotic form is $\text{const. } \sin(Kr - (1/2)\ell\pi)$ so that the logarithmic derivative depends only on whether ℓ is even or odd. As long as this is the case, the eigenvalues depend only on whether ℓ is even or odd, regardless of the shape of the potential near the nuclear surface, provided only that KR , where K is the wave number inside the nucleus and R the radius. This condition is violated only for rather high ℓ , for which, in other words, the centrifugal force is still comparable with the well depth at the nuclear surface, and such states do not contribute much to the effects we are considering.

Hence, in general, the only terms with small denominators in Eq. (71) come from states in which the extra particle has lost a considerable

amount of energy to the target nucleus, and in which the probability of further energy transfer is considerably reduced.

An exception to this is the case in which the particle makes a transition to a state with practically the same energy. This may either be a different substate for the same l , i. e., a change in direction of the angular momentum, or a transition from an even to another even or an odd to an odd state, since, as we have seen, these lie close together. This requires that the target nucleus also change its angular momentum, and to obtain a small energy denominator, we must require the target nucleus to have low-lying excited states, with different angular momenta. This complication is connected with the possible existence of rotational states in the target nucleus, when the use of a spherical potential well is no longer justified. In such cases the right procedure is to introduce a deformed well for the optical potential, and this makes it possible to eliminate the off-diagonal elements of the interaction between states of practically the same energy.

The general conclusion from this discussion is that we have in Eq. (71) a definition of the optical potential of which we can see that it yields a good approximation to the average scattering amplitude with the averaging interval B being less than the width of the giant resonance.

However, in this form the expression is not suitable for a practical calculation of the optical potential, in particular of its imaginary part, since it would require the knowledge of the exact wave functions of many excited states of the target nucleus.

One can estimate the absorption coefficient by using, instead of the exact eigenstates of the target nucleus, the wave functions of non-interacting particles, i. e., the shell model approximation. As we saw in the first section of these lectures this is a reasonable approximation for the ground state. It will not be a good approximation for an individual excited state, except for very low excitation, but Eq. (71) is insensitive to the mixing of the different states of the target nucleus for the same reason that we have found it insensitive to the mixing of compound states. However, the cruder approximation to the denominator of Eq. (70) which such an approach involves restricts one to a larger value of the interval B .

Such calculations for the imaginary part of the potential for infinite nuclear matter have been carried out by several authors, the most careful one being probably that of Shaw (private communication from Prof. Bethe), and one finds a value rather less than required for empirical fits of optical potentials.

The reason for this discrepancy is probably that in empirical fits one usually assumes the imaginary part of the potential to have the same shape as the real part, i. e., more or less constant inside the nucleus and then dropping off at the surface. There are, however, reasons to expect that the absorption is, in fact, stronger near the surface than in the interior; and, since the empirical fits are not too sensitive to the exact shape, the comparison therefore overestimates the absorption in the interior.

One expects an increased absorption near the surface mainly from the fact that the absorption, i. e., the energy transfer to the target nucleons, is inhibited at high density by the Pauli principle, by which only few nucleons can accept small amounts of energy. If the surface region can be regarded as a region of lower density, the Pauli principle should therefore be less important. The same point can be made by noting that near the surface there is an appreciable gradient of the potential, and therefore one must no longer impose conservation of momentum on the collision of two nucleons. They may now exchange momentum with the potential well, i. e., with the nucleus as a whole. This alters the restrictions on the permissible processes.

These qualitative arguments make it appear likely that an evaluation of Eq. (71) for a finite target nucleus would, in fact, yield an imaginary part which is peaked near the surface. In addition, if the excitation of low-lying collective states (rotational or vibrational) is of any importance for the energy transfer to the target, this would be expected to be strong in the surface region.

This effect, too, is in principle contained in Eq. (71) if we use the exact eigenstates for the target, but it will be lost if we treat these in a shell-model approximation.

Similar arguments can be applied to inelastic scattering into states of low excitation, starting most conveniently from Eq. (59). Again it can be shown that the last term is small on the average, so that the average amplitude is given by the second term in Eq. (59) (the first being zero if $a \neq b$) which is of the form of first-order Born approximation. One is therefore led to the "direct interaction" picture for the average inelastic amplitude.

It should, of course, be remembered that throughout this section we have treated the incident nucleon as distinguishable from the target nucleons and have therefore neglected exchange effects. We have also assumed that the matrix elements of the interaction potential between uncoupled states are of a reasonable order of magnitude, and thus excluded forces with hard cores. Further developments of the formalism are therefore required to cover these two points, but it is not likely that they will affect the general nature of the results.

III. Collective Degrees of Freedom in the Nucleus

We now turn from the shell model and the optical model to the problem of collective motion, which, in the hands of A. Bohr and Motelson has proved a very useful tool in understanding many interesting features of nuclear physics, particularly concerning the low-lying states of nuclei with large, partly-filled shells. Of the collective types of motion the rotational states are probably the most pronounced, but vibrational states are also of importance, and we shall later see that it is useful also to regard the motion of the center of mass as a collective degree of freedom; it is the simplest of all.

The problem of whether nuclei can rotate gave rise to speculation as

early as the 1930's. If one pictures a nucleus naively as rotating like a rigid body, its rotational states should correspond to excitation energies which, for the heavier nuclei, would be very low, corresponding to their fairly large moments of inertia. Such low-lying states had not been noticed at that time, and it was not clear whether or not they ought to exist.

To understand what is involved here, consider the very simple problem of two particles moving on a circle. If they do not interact, and if they are distinguishable, so that wave functions of any symmetry are permissible, then the lowest state must have angular momentum zero, and the first state of one unit of angular momentum is obtained by exciting one particle. Its energy is

$$\hbar^2/2ma^2$$

where m is the mass of a particle, and a the radius of the circle. There are two states of this angular momentum, because we can excite either particle.

If the particles attract each other sufficiently strongly to form a bound state, the excitation energy is reduced to

$$\hbar^2/4ma^2$$

corresponding to the moment of inertia of the two tied particles. The result is the same if the particles repel each other strongly, so that they tend to be on opposite ends of a diameter.

However, if the particles are identical, obeying either Bose or Fermi statistics, then the answer is essentially dependent on whether the forces are repulsive or attractive. For attractive forces it is as above, but for repulsive forces the particles tend to form a configuration for which an exchange of the particles is identical with a rotation through 180 degrees. Since an eigenfunction of even (odd) angular momentum is even (odd) under a rotation through 180 degrees, only even rotational states are permitted for Bose, and odd states for Fermi statistics. Thus, for example, in the case of bosons the lowest rotational state has energy

$$\hbar^2/ma^2$$

which is higher than for noninteracting particles.

These results for two particles are easily verified by explicit calculation, but it is not easy to see how they generalize to the case of many particles. If in the many-body case the forces are strong enough to keep the particles in or near a definite equilibrium configuration, we have the situation which is usually found in molecules. The rotational states are then those of a rigid body, except that again the symmetry of the equilibrium configuration may result in certain states being prohibited. For example, if we consider a benzene molecule (whose wave function is symmetric in the coordinates of the carbon atoms) rotating in its own plane,

a rotation by 60 degrees is equivalent to a cyclic interchange of the atoms, and in consequence, only every sixth rotational state is allowed.

We know, however, that nuclear forces are not strong enough to keep the nucleons in any particular configuration; the zero-point amplitude of their vibrations about their relative equilibrium positions would exceed their average distance. It is likely, however, that they will with high probability be in patterns corresponding to a fairly uniform distribution. If such a pattern is rotated through a small angle, it leads to a configuration which is not far from one which can be obtained from the original one by an interchange of nucleons.

Such considerations were used by Teller and Wheeler,²⁴ who conjectured that one should not expect to find rotational states of low energy.

Much later, Bohr and Mottelson²⁵ started from the idea that nuclei with partly filled large shells should be pictured as nonspherical in shape. The reason is that the nucleon-nucleon forces are, on balance, attractive. If several nucleons move in orbits of large orbital angular momentum the most favorable arrangement is one in which the axes of their orbits are parallel, so that their orbits stay as close to each other as possible. This means that the self-consistent field, which represents the action of all other nucleons on a given one, becomes appreciably anisotropic.

This argument was invoked by Rainwater²⁶ to explain the static quadrupole moments of nuclei. The situation is the opposite to that in the atom, where the interaction between the electrons is repulsive, so that even in large unfilled shells the electronic orbits always arrange themselves so as to keep the average charge distribution as isotropic as possible.

Bohr and Mottelson went further in treating the parameters which determine the potential field as physical variables. These parameters comprise in particular the distortion of the nucleus, i. e., its deviation from a spherical shape, and its orientation. If these are treated as physical degrees of freedom, they evidently lead to surface vibrations and to rotations.

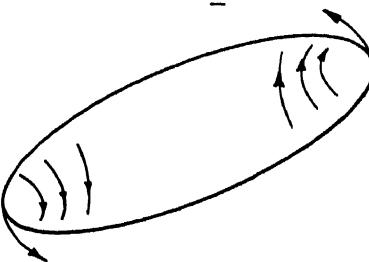
This approach has been so fruitful in the interpretation of experiments that there is no doubt that the underlying concepts are significant parts of the physical situation. The question arises, therefore, how one can relate this description to the basic many-body problem, and how, at least in principle, one is to calculate the parameters from the basic nuclear forces and from other nuclear properties. One of the interesting parameters here is the moment of inertia, which governs the spacing of rotational levels.

Many nuclei show series of states for which energy and angular momentum are related by

$$E = \frac{k^2}{2I} j(j+1) \quad (72)$$

where I may therefore be interpreted as a moment of inertia. For even nuclei, for which the spins of the nucleons cancel in the ground state, only even j occur; and the first two excited levels therefore have $j = 2$ and 4, and their energies, measured from the ground state, are in the ratio 3:10.

The simplest picture one might consider for this is to think of the nucleus as nonspherical in shape, and allow the external surface to rotate. The nuclear matter inside this surface then must also move, since its normal velocity at the surface must equal the normal velocity of the surface itself. As is well known, this requirement does not determine the velocity distribution uniquely. One possible hypothesis is to assume that the flow is irrotational, so that $\text{curl } \underline{u} = 0$. This leads to streamlines



roughly as shown in the diagram. The amount of flow which takes place then depends on the degree of anisotropy of the surface. For a spherical surface \underline{u} vanishes everywhere, and for small anisotropy the velocity is correspondingly small. Bohr and Mottelson estimated the resulting "irrotational" moment of inertia, taking the anisotropy from observations of electric quadrupole moments, and found that it is much smaller than the values required to fit the rotational levels. The latter require a moment of inertia of the order of that of a rigid nucleus, perhaps one-half the rigid value.

A rather more sophisticated approach is based on the "cranking model" proposed by Inglis,²⁷ and elaborated by Bohr and Mottelson,²⁸ in which one assumes an anisotropic potential field which rotates about a given axis with an externally given angular velocity, and then calculates the energy of nucleons moving in this rotating field. In the simplest variant of this model, in which the nucleons do not interact, one obtains exactly the rigid moment of inertia.

This can be seen without any calculation from the remark that the effect of a rotating coordinate system is equivalent to the effect of a magnetic field of which the Larmor period equals the period of revolution, except for the centrifugal force term

$$\frac{1}{2} m \omega^2 r^2$$

for each particle, where ω is the angular velocity and r the distance from the axis of rotation. Now it is known that the diamagnetism of a gas of free particles is very small--it vanishes in the classical limit--so that

the main effect of the rotation on the energy is in that case given by the centrifugal force term. If this is averaged over all particles, one obtains an energy

$$\frac{1}{2} I \omega^2$$

where I is the classical moment of inertia of the average mass distribution.

It is probable that the interaction between the particles would reduce this moment of inertia and thus bring it nearer to the observed value. It is not easy, however, to take this interaction into account consistently, since the potential well, which, as we saw, represents the average interaction between the nucleons in some sense, allows already for some of this interaction, so that one cannot clearly define the residual interaction unless one can, in fact, derive the potential well from the forces. One needs therefore a description in which the rotating well appears naturally from the many-body problem.

Many attempts have been made to give a consistent formulation of the dynamical problem which includes the collective features which are intuitively clear, and whose existence is confirmed by experiment. The problem is difficult for the following reason: one wants to introduce variables which represent, for example, the shape, i. e., the anisotropy of the nucleus, and its orientation. Since we are interested in their variation with time we must treat them as dynamical variables, and they must therefore appear in a wave function. Thus we might expect to use a wave function of the form:

$$\Psi(\Theta, \phi, \psi; \alpha, \beta, \dots; r_1, r_2, \dots, r_N) \quad (73)$$

where Θ, ϕ, ψ are the Euler angles, α, β, \dots are deformation parameters, and the rest are the particle coordinates.

But this cannot be right, since our problem has only $3N$ degrees of freedom and the number of variables in the wave function cannot exceed this number. One way out would be to regard the collective variables in Eq. (73) as functions of the nucleon coordinates; this could be done by defining the instantaneous inertia tensor of the particle distribution and then connect the shape and orientation with the principal values and principal axes of this tensor. Such a treatment would, however, lead to very complicated equations in which the dynamics of the collective motion would be quite obscure.

An alternative is to replace the particle coordinates in Eq. (73) by a new set of $3N - n$ functions of the coordinates, where n is the number of collective variables, so that the new variables are all independent, e. g.,

$$\Psi(\Theta, \phi, \psi; \alpha, \beta, \dots; \tilde{r}_1, \dots, \tilde{r}_{3N-n}) \quad (74)$$

One would then like the $\vec{\Psi}$ to have some similarity to particle coordinates, since many of the features of such nuclei seem to call for single-particle excitations as in the shell model, in addition to collective excitations.

We should, after this transformation, expect to find the Hamiltonian in the form

$$H = H_{\text{COUL}} + H_{\text{INT}} + H_{\text{COUP}} \quad (75)$$

where the first term operates only on the collective variables and represents the energy of a rotating and oscillating body. The second term acts only on the internal variables, and has a constant value if only rotations and oscillations are excited with the internal degrees of freedom in their normal state. The last term is the remainder which couples collective and internal motion.

It is, of course, always possible to write any Hamiltonian in the form Eq. (75); in fact, one may prescribe the first two parts arbitrarily, since the last term depends on all variables. But the procedure is useful only if one knows that the coupling term is small, so that to some approximation one can describe the problem in terms of collective and particle excitations separately. Of many ingenious attempts in this direction none has yet led to a form in which the smallness of the coupling term can be demonstrated.

A modification of this procedure is to leave redundant variables in the description, but to add subsidiary conditions which appropriately reduce the number of independent variables. In finding approximate solutions to the equations, one need not then enforce the subsidiary conditions rigorously, but only to the accuracy to which one solves the equations. The difficulties in obtaining a form of the theory in which the corrections to the simple collective model can be shown to be small seem to be just as serious as with the other procedure.

I shall describe here an alternative approach which avoids some of these complications. I should stress that here, too, not all the difficulties have been overcome, so that this third section of the lecture course represents a progress report rather than a presentation of final answers.

The general principle from which we shall start was used in very similar ways by Hill and Wheeler,²⁹ Redlich and Wigner,³⁰ Griffin and Wheeler,^{31, 32} and Peierls and Yoccoz.³³

Assume for simplicity that the forces contain no repulsive cores, so that we may start in the spirit of the Hartree-Fock approximation, without the refinements discussed in section I above. In other words, we start from the expression for the energy:

$$E = \frac{\langle \vec{\Phi}^* H \vec{\Phi} \rangle}{\langle \vec{\Phi}^* \vec{\Phi} \rangle} \quad (76)$$

where Ψ is again a Slater determinant of one-particle eigenfunctions for a suitable potential well U , which may be velocity-dependent. It is then clear from Rainwater's argument that for an incomplete shell of appreciable orbital angular momentum it may be favorable to make the potential well anisotropic. In that case the function Ψ in Eq. (76) depends on the shape and orientation of the well; the energy will depend on the shape but evidently not on the orientation.

Assume therefore that the energy Eq. (76) has been minimized so as to give the optimum shape of the well. (Thereby we exclude collective vibrations, for which one has to consider shapes different from, though close to, the optimum.) Then everything is in principle determined, except the orientation of the well U , and consequently, of the wave function Ψ .

For simplicity of notation, assume for the moment that the problem is two-dimensional; the orientation is then specified by a single angle, Θ . We are now faced with a degeneracy in the sense that there exists a family of trial functions which all give the same expectation value of the energy. It is well known that in that case one can lower the energy further, and hence improve the approximation by choosing a linear combination of these degenerate functions. Since our degenerate functions form a continuous family, the linear combination is an integral:

$$\Psi(x) = \int f(\theta) \Phi_\theta(x) d\theta \quad (77)$$

where the coefficient $f(\theta)$ is arbitrary. We now determine this coefficient by the requirement that the energy be a minimum. Inserting Ψ as a trial function in Eq. (76) and varying with respect to f , we find after some straightforward transformations

$$E = \frac{\int d\theta d\theta' f^*(\theta) f(\theta') h(\theta - \theta')}{\int d\theta d\theta' f^*(\theta) f(\theta') n(\theta - \theta')} \quad (78)$$

which is stationary when

$$\int [h(\theta - \theta') - E n(\theta - \theta')] f(\theta') d\theta' = 0. \quad (79)$$

Here

$$\begin{aligned} h(\theta - \theta') &= \langle \Phi_\theta^* H \Phi_{\theta'} \rangle \\ n(\theta - \theta') &= \langle \Phi_\theta^* \Phi_{\theta'} \rangle . \end{aligned} \quad (80)$$

The fact that h and n are functions of the difference between the angles only is a consequence of the isotropy of the complete Hamiltonian H .

It is now evident that the correct solution for f , apart from a constant factor, is

$$f = e^{im\theta} \quad (81)$$

where m must be an integer. If our potential well, U , had a center of symmetry, the Slater function Ψ_0 will be even or odd under rotations through 180° , and therefore the trial function Eq. (77) exists only for even or odd m , respectively.

With this choice of f , the trial function Ψ is an eigenstate of the total angular momentum, as is the case for the exact solution to the many-body problem, but not for the Slater determinant based on an anisotropic well. In fact, the transformation Eq. (77) with f given by Eq. (81) is just a projection on the states of angular momentum m .

Now, if the nucleus contains many particles and is appreciably anisotropic, the function h and n decrease very rapidly as the angle difference increases. Defining moments

$$n_\mu = \int n(\theta) \theta'' d\theta, \quad h_\mu = \int h(\theta) \theta'' d\theta$$

of which the odd ones vanish, we find to a good approximation

$$E = \frac{h_0 - \frac{1}{2}m^2 h_e}{n_0 - \frac{1}{2}m^2 n_e} = \frac{h_0}{n_0} + \frac{1}{2}m^2 \left(\frac{h_e n_e}{n_0^2} - \frac{h_0}{n_0} \right) + \dots \quad (82)$$

It is easy to see that the higher terms neglected in Eq. (82) are small just in the circumstances when the rotational model is well confirmed by experiment, i. e., for large deformation and not too large rotational angular momentum.

This method can easily be applied to the three-dimensional rotation of an axially symmetric well, and the only change is that in Eq. (77) there is an integration over two angles, and f becomes a spherical harmonic. In the energy expression Eq. (82), m^2 is replaced by $j(j+1)$. The method can also be generalized to cases in which one expects the well to be deformed unsymmetrically, and to surface oscillations.

The coefficient of m^2 in Eq. (82), or of $j(j+1)$ in the three-dimensional case is then related to the moment of inertia. One might therefore expect that it should be possible to estimate the moment of inertia of nuclear rotation in this way. Such calculations were carried out by Yoccoz³⁴ using Yukawa forces between the nucleons, and an anisotropic harmonic oscillator potential to generate the trial wave function Ψ , i. e., neglecting spin-orbit coupling and not using complete self-consistency. The results gave a moment of inertia of the order of, but

rather less than, the rigid value, and agreeing for various nuclei as well with the observed values as could be expected for such a crude model.

There is, however, reason to doubt whether the moments of inertia obtained in this way are reliable. This is because we may apply the same technique to the motion of the center of mass of the nucleus, which is also a collective motion, and in this way, calculate the translational kinetic energy. Since we know the correct answer for this, it forms a check on the validity of the method, and, as we shall see, the answer is unsatisfactory.

It is instructive, first of all to consider the problem of center-of-mass motion in a specially simple case. We know, of course, always how to separate the coordinate of the center of mass from the internal coordinates, but usually the problem of the internal motion then no longer resembles the problem of independent particles, and we do not know how to connect this procedure with shell-model calculations.

The shell model itself starts from the fiction of an external potential acting on all particles, and therefore trying to locate also the center of mass. The excited states then include the possibility of the center of mass oscillating under the influence of this force, and such oscillations have no reality.

Skyrme and Elliott³⁵ noticed that these spurious excitations can be eliminated in the particular case of a harmonic well. In this case the wave function for any non-degenerate state is already factorized in two parts of which one depends only on the center-of-mass coordinate, and the other on the internal coordinates. For instance, if we take N spin-less fermions in one dimension the Slater determinant is of the form

$$\begin{vmatrix} 1 & 1 & \dots & 1 \\ x_1 & x_2 & \dots & x_N \\ h_1(x_1) & h_1(x_2) & \dots & h_1(x_N) \\ \dots & \dots & \dots & \dots \\ h_{N-1}(x_1) & h_{N-1}(x_2) & \dots & h_{N-1}(x_N) \end{vmatrix} e^{-\frac{\alpha}{2} \sum x_i^2} \quad (83)$$

Here, apart from a constant factor, each Hermite polynomial h_n may be replaced by the highest power it contains, since the rest is always a multiple of another row of the determinant so that the determinant may be replaced by

$$\begin{vmatrix} 1 & 1 & 1 & \dots & 1 \\ x_1 & x_2 & x_3 & \dots & x_N \\ x_1^2 & x_2^2 & x_3^2 & \dots & x_N^2 \\ \dots & \dots & \dots & \dots & \dots \\ x_1^{N-1} & x_2^{N-1} & x_3^{N-1} & \dots & x_N^{N-1} \end{vmatrix} .$$

This is clearly a function of the internal variable only, since the addition of a constant displacement to all adds to each row only multiples of other rows and therefore does not change the determinant. Thus the dependence on the center-of-mass coordinate is contained in the exponential factor.

Define

$$\bar{x} = \frac{1}{N} \sum x_i$$

and

$$\xi_i = x_i - \bar{x}$$

Then

$$\sum_i x_i^2 = \sum_i \xi_i^2 + N \bar{x}^2$$

so that

$$e^{-\frac{\alpha}{2} \sum_i x_i^2} = e^{-\frac{\alpha}{2} \sum_i \xi_i^2} e^{-\frac{\alpha}{2} N \bar{x}^2}.$$

Now the first factor depends only on the relative positions of the nucleons, and the second represents the spurious oscillations of the center.

Now consider a wave function obtained by multiplying Eq. (83) by

$$(x_1 + x_2 + x_3 + \cdots + x_N).$$

It is easily seen that this is again an eigenfunction of the independent-particle model in the harmonic well, with an excitation energy of one quantum of oscillation. Looked at as a function of each individual particle coordinate it is very similar to the shell model wave functions; yet we have multiplied Eq. (83) simply by a multiple of the center-of-mass coordinate \bar{x} , and therefore the wave function of the internal motion is unchanged, and only the ground state of the center-of-mass oscillation has been replaced by the first excited state.

In other words, this is a nucleus in its ground state, oscillating as a whole in the spurious well, and therefore does not represent any state of the real nucleus. Skyrme and Elliott showed that a state of this kind occurs in the shell-model analysis of O^{16} , which should, of course, be discarded. Oddly enough, there exists a level of appropriate symmetry in the observed spectrum of O^{16} , though at rather higher energy than expected from the shell model. Whether this may, after all have some relation to this spurious level, or whether by accident there arises such a level from a different configuration, is not yet completely clear.

The exact factorization of the wave function is possible only for the harmonic oscillator well. The procedure outlined for the rotational

states may, on the other hand, be applied generally. The analog or Eq. (77) is now

$$\Psi(x) = \int e^{ikr} \Phi(x-r) dr \quad (84)$$

where we have already used the fact that the optimum choice of the coefficient f must now be exponential in the displacement r .

We expect, of course, that the energy will be of the form

$$E = E_0 + \frac{1}{2mN} k^2 \quad (85)$$

where m is the mass of one nucleon. We can formally establish this by remarking that the exact wave function of the nucleus must be of the form

$$\Psi_{\text{EXACT}} = e^{ik\bar{x}} \chi(x-\bar{x}) \quad (86)$$

where χ depends only on the relative coordinates. It is easy to show from the Schrödinger equation that the energy of this function is of the form Eq. (85), provided that the internal eigenfunction χ is independent of k .

If we multiply Eq. (84) by $e^{-ik\bar{x}}$ we can define again a function

$$\chi(x-\bar{x}) = \int e^{ik(r-\bar{x})} \Phi(x-r) dr \quad (87)$$

which allows us to put our trial function into a form like Eq. (86). Eq. (87) is again a function of the relative coordinates only, but it is not independent of k . (It would be if χ were always equal to r , i. e., if the center of mass of the particles always coincided with the center of the well. For a large number of particles this is approximately true, but not exactly.)

We therefore cannot draw any simple conclusion about the translational energy from our trial function, but have to evaluate it. This evaluation is rather difficult for fermions, but it is instructive to carry it out for bosons, for which the problem of the center-of-mass motion ought not to be very different. One easily shows that the expression for the energy is

$$E = \frac{\int e^{-ikr} \langle \Phi^*(x-r) H \Phi(x) \rangle dr}{\int e^{-ikr} \langle \Phi^*(x-r) \Phi(x) \rangle dr} \quad (88)$$

For the ground state of the boson system for which all particles are in the same state, say $u(x)$, we have for the denominator:

$$D = \int e^{-ikr} dr \left[\int u^*(x-r) u(x) dx \right]^N. \quad (89)$$

The overlap integral

$$\int u^*(x-r) u(x) dx$$

is unity for $r=0$, and will decrease with increasing r being negligible when r is substantially larger than the extension of the wave function $u(x)$. Its N -th power will therefore decrease much more rapidly and will be negligible when r is only $N^{-1/2}$ times the extension of the one-particle wave function. We therefore require the integrand of Eq. (89) only for small r , and there we may in the overlap integral expand $u^*(x-r)$ in a Taylor series. Since the linear term vanishes by symmetry we find easily for the overlap integral

$$1 - \frac{1}{2} r^2 (p^2)_{\text{oo}} = 1 - \frac{1}{2} r^2 \alpha$$

where the last factor is the diagonal matrix element of p^2 for the ground state of one particle.

Then

$$(1 - \frac{1}{2} r^2 \alpha)^N \sim e^{-\frac{1}{2} N \alpha r^2}$$

and

$$D = \int e^{ikr - \frac{1}{2} N \alpha r^2} dr = \sqrt{\frac{2\pi}{N\alpha}} e^{-k^2/2N\alpha}$$

The corresponding treatment of the denominator is rather more long-winded. It leads, however, to the result that the integrand is also a Gaussian function of r . If we accept this result without proof, the rest of the calculation is straightforward.

Let

$$\langle \Phi^*(x-r) H \Phi(x-r) \rangle = A e^{-\frac{1}{2} N \beta k^2} \quad (90)$$

For $r=0$, this is just the expectation value of H for the shell model wave function Φ , and thus equal to the shell model approximation for the energy, $A = E_0$.

Differentiating both sides of Eq. (90) twice with respect to r and then setting $r = 0$, we find

$$-N\beta A = -\langle \Phi^* P^2 H \Phi \rangle$$

where P is the total momentum of all particles. Inserting all these results in Eq. (88) and carrying out the integration:

$$E = E_0 \sqrt{\frac{\alpha}{\beta}} e^{+\frac{k^2}{2N}(\frac{1}{\alpha} - \frac{1}{\beta})} = E_0 \sqrt{\frac{\alpha}{\beta}} \left(1 + \frac{k^2}{2N}(\frac{1}{\alpha} - \frac{1}{\beta}) + \dots\right)$$

Neglecting the difference between α and β , which is small of order $1/N$, we have

$$E = E_0 + \frac{k^2}{2} \frac{\langle P^2 H \rangle - \langle P^2 \rangle \langle H \rangle}{\langle P^2 \rangle^2} \quad (91)$$

where the brackets indicate expectation values for the ground state wave function of N particles. Consider first the contribution to Eq. (91) of the kinetic energy part of the Hamiltonian (which for the exact wave function would give the whole of the translational energy). This easily reduces to

$$\frac{k^2}{4Nm} \frac{\langle p^4 \rangle - \langle p^2 \rangle^2}{\langle p^2 \rangle^2} \quad (92)$$

where the averages are taken for one particle.

In the particular case of a harmonic well the momentum distribution is Gaussian, so that

$$\langle p^4 \rangle = 3 \langle p^2 \rangle^2.$$

In that case Eq. (91) therefore gives the correct translational energy. This is not surprising since for the harmonic oscillator the shell model function factorizes like Eq. (83), except that the determinant factor is absent in the boson case, so that the operation Eq. (84) acts only on the center-of-mass coordinate, leaving the internal part alone, so that our trial function then is actually of the required form Eq. (86) with a k -independent internal wave function.

It is equally clear that for a potential well of different nature, with a different momentum distribution the answer must, in general, be different by a numerical factor.

The same is true if we use the total Hamiltonian, potential and kinetic energy, in Eq. (91). We then obtain integrals involving the two-body potential $v(x_i - x_j)$. If we assume that the potential well is the self-consistent potential belonging to this interaction, we can eliminate the

two-body forces and obtain by fairly simple manipulation for the total energy:

$$E = \text{const.} + \frac{k^2}{8N} \frac{\langle \partial^2 U / \partial x^2 \rangle}{\langle p^2 \rangle^2} .$$

This again gives the correct answer for the harmonic oscillator potential, but not otherwise.

These discrepancies do not necessarily imply that our trial function is very bad. One has to remember that we are dealing with a large number of particles (otherwise the shell model approximation would not be reasonable) and that the leading term in the energy is proportional to N (if we arrange to keep the density independent of N). Hence the translational energy which is proportional to $1/N$, is compared to the leading term, small of second order on the parameter $1/N$. In a sense, it is therefore already an achievement to get this to be of the right order of magnitude and wrong only by a numerical factor.

However, it is clear that the method as it stands is not adequate to calculate the translational energy, and we therefore cannot trust it either for the very similar problem of rotation, unless we could test its validity for that case, in which we have, of course, no independent knowledge of the answer.

The question therefore arises whether it is possible to improve our trial function sufficiently to obtain a better value for the translational or rotational energy and, at the same time, estimate the error. Since the only error in the trial function arises from the fact that we have replaced the two-body interaction

$$V = \sum_{i < j} V_{ij}$$

by the effect of a potential well

$$U = \sum_i U_i$$

it is natural to consider the difference

$$W = V - U \quad (93)$$

as a small perturbation. The success of the shell model and the fact that the trial function gives the translational energy right in order of magnitude may be regarded as encouraging indications for this.

There are, in principle, two ways in which we may try to allow for the effect of the perturbation. The first, and perhaps the most obvious, would be to replace in Eq. (84) the Slater determinant Φ by a

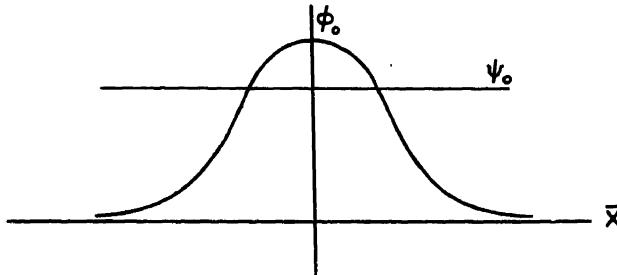
perturbation series

$$\Phi = \Phi_0 + \Phi_1 + \Phi_2 + \dots \quad (94)$$

sorted in powers of the perturbation Eq. (93). In other words, we use the kind of perturbation theory which was discussed at the beginning of the first section of this course and apply the operation Eq. (84) which projects on a given eigenvalue of the total momentum.

However, this procedure is not satisfactory, since one can see that the series Eq. (94) cannot converge usefully. Indeed, if it did converge, it would tend to a solution of the exact problem, which would already be a momentum eigenstate, so that the projection would be redundant. Since we start from the ground state of the unperturbed system, the perturbation theory, if convergent, would lead us to the state of lowest energy of the perturbed system, i. e., a nucleus in its ground state at rest.

Consider now the dependence of the unperturbed wave function Φ and of the exact solution Ψ on the center-of-mass coordinate \bar{x} , for fixed relative positions of the particles. The first is the solution of a problem in which there is a definite equilibrium position for the center of mass. The second belonging to total momentum zero, is independent of \bar{x} . (See figure.) It is clear that we cannot go from one to the other by a perturbation expansion. This situation applies generally when we try to go from a discrete state to the edge of a continuous spectrum.



At first sight this result might make all shell model calculations which are based on the series Eq. (94), or refinements of it, appear suspect. However, it must be remembered that in practice one never carries out the infinite summation but breaks the sum off after a few terms. At this stage we may expect to have improved our description of the internal motion considerably, but we cannot expect to approach the correct answer for the motion or energy of the center of mass. However, in most of the usual applications we are not interested in the center-of-mass motion and its contribution to the total energy, and even to the relative position of various excited states, is likely to be quite small, as we have seen. For the usual problems of nuclear structure the point is

therefore academic. But for our present purpose of studying the center of mass and other collective problems, it is evidently of importance.

The situation is well illustrated by taking the harmonic oscillator problem literally. If we want the self-consistent potential to be harmonic, we must choose also harmonic forces between the particles. To simplify our algebra further we shall assume we are dealing with bosons. If we assume

$$V = \frac{1}{2} \beta \sum_{i < j} (x_i - x_j)^2 \quad (95)$$

we see easily that the self-consistent field, apart from a constant, is

$$U(x) = \frac{1}{2} \beta (N-1) x^2 \quad (96)$$

so that the solution in the shell model approximation is

$$\Phi_0 = \text{const. } e^{-\frac{1}{2} \sqrt{\beta N} \sqrt{N-1} \sum_i x_i^2}. \quad (97)$$

In this academic case we can solve the many-body problem exactly. We may write the potential exactly as

$$V = \frac{1}{2} \beta N \sum_i x_i^2 - \beta (Nx)^2 \quad (98)$$

which differs from the single-particle potential for which we have solved the equation firstly by the coefficient of the first term being N in place of $(N-1)$, and secondly by the second term, which removes the force on the center of mass.

Now, as we noted previously, the problem of many particles in a harmonic well, as well as the exact problem is separable as between center of mass and internal variables. The internal potential of Eq. (98) is the same as that of the first term alone. We may therefore solve the problem with the one-particle potential

$$\frac{1}{2} N \beta \sum_i x_i^2$$

and from its solution remove the factor depending on \bar{x} , and replace it by

$$e^{ik\bar{x}}$$

as appropriate to free motion.

Thus, the exact solution is found to be

$$\begin{aligned}\Psi_0 &= \text{const. } e^{-\frac{1}{2}\sqrt{\beta m}/N(\sum_i x_i^2 - N\bar{x}^2) + ik\bar{x}} \\ &= \text{const. } e^{-\frac{1}{2}\sqrt{\beta m}/N \sum_i \xi_i^2 + ik\bar{x}}\end{aligned}\quad (99)$$

where, as before, we have put

$$\xi_i = x_i - \bar{x}$$

By comparison, the shell-model function Eq. (97) may be written as

$$\Phi_0 = \text{const. } e^{-\frac{1}{2}\sqrt{\beta m}/N-1 \sum_i \xi_i^2 - \frac{1}{2}\sqrt{\beta m}/N-1 N\bar{x}^2}. \quad (100)$$

It is now possible to see what would happen if we applied the perturbation theory to get from Eq. (100) to Eq. (99). Since both the unperturbed and the exact problem are separable, the perturbation may be divided into two parts, which act on the center of mass and on the internal variables, respectively. As regards the center of mass, we start from an unperturbed potential

$$U_0 = \frac{1}{2} \beta N(N-1) \bar{x}^2$$

and add a perturbation which is equal and opposite to it. To generate the perturbation series, we multiply the perturbation by a parameter λ , so that we have to solve the problem with the potential

$$(1 - \lambda) U_0$$

and mass Nm which has ground-state energy

$$\frac{1}{2} \sqrt{\frac{\beta}{m}} \sqrt{N-1} \sqrt{1-\lambda} .$$

Perturbation theory gives us this result expanded into powers of λ . We require this for the value $\lambda = 1$, which is just on the radius of convergence of the series.

Consider, on the other hand, the internal factors of Eqs. (99) and (100). These differ merely by having

$$\sqrt{N}$$

and

$$\sqrt{N-1}$$

respectively, in the exponent. Clearly it is in order to expand the difference, so that we may write the exponent of Eq. (99) as

$$\frac{1}{2} \sqrt{\beta m} \sum_i \xi_i^2 \left\{ \sqrt{N-1} + \frac{1}{2} \frac{1}{\sqrt{N-1}} - \dots \right\}$$

and this series converges well as long as N is large. This suggests writing the exponential as

$$e^{-\frac{1}{2} \sqrt{\beta m} \sqrt{N-1} \sum_i \xi_i^2} \left(1 - \frac{1}{4} \sqrt{\beta m} \frac{1}{\sqrt{N-1}} \sum_i \xi_i^2 \right)$$

but here one sees easily that the mean value of the second term is of the same order as the leading term, which looks dangerous. However, it is obvious that this is the "unlinked cluster" trouble which was discussed in the first section. It requires caution, but does not necessarily invalidate a perturbation approach to the energy.

To return to the general problem, it is now clear that the procedure based on the perturbation series Eq. (94) is not acceptable. Instead, we may form a momentum eigenfunction from each solution (ground state and all excited states) of the independent-particle model:

$$\Psi_n = \int e^{ikr} \Phi_n(x-r) dr \quad (101)$$

and thus obtain an infinite set of functions which is still complete, in the sense that an arbitrary function of total momentum k can be expanded in a series

$$\Psi = \sum_n c_n \Psi_n \quad (102)$$

but this expansion is now no longer unique, since the states Eq. (101) are neither independent nor orthogonal.

This can be seen from the fact that the set Ψ_n contains the same number of functions as the set of the Φ_n in the sense that there is a one-to-one correspondence but they can describe only the subspace belonging to a momentum eigenvalue. The most trivial example would be that of a single particle, $N = 1$, for which all the functions Eq. (101) are proportional to e^{ikx} , and we are using an infinite set of function where only one is required.

We now try to choose the coefficients in Eq. (102) in such a way that the series solves the exact Schrödinger equation. By inserting Eq. (102) into the variation principle, it is easy to show that the condition for the coefficients becomes

$$\sum_l \{N_{nl}(E - E_l) - W_{nl}\} c_l = 0 \quad (103)$$

where E_l is the l -th eigenvalue of the independent-particle problem, and

$$\begin{aligned} N_{nl} &= \int e^{-ikr} \langle \Phi_n^*(x-r) \Phi_l(x) \rangle dr \\ W_{nl} &= \int e^{-ikr} \langle \Phi_n^*(x-r) W(x) \Phi_l(x) \rangle dr, \end{aligned} \quad (104)$$

W being the difference between two-body potential and potential well, as before.

In this form it looks much more hopeful to try perturbation theory, since all our functions already have the correct dependence on the center-of-mass coordinate, so that the previous objection no longer applies.

We therefore expand the eigenvalue E and the coefficients c_n in a series:

$$E = E_0 + \epsilon^{(1)} + \epsilon^{(2)} + \dots$$

$$c_n = \delta_{n0} + c_n^{(1)} + c_n^{(2)} + \dots$$

of successive orders of approximation. Treating the W_{nl} in Eq. (103) as small of first order, we find to first order

$$\sum_l N_{nl}(E_0 - E_l) c_l^{(1)} = W_{n0} - \epsilon^{(1)} N_{n0} \quad (105)$$

and similarly in higher orders.

However, Eq. (105) is not yet sufficient to define our approach completely. The redundancy of our expansion has the consequence that the inhomogeneous Eq. (105) admits a great variety of solutions. This would be unimportant if different solutions gave us simply different expansion coefficients for the same first-order wave function. This, however, is not the case. The reason can be seen as follows:

The series of approximations of which Eq. (105) is the beginning is essentially a perturbation theory in which we have divided the Hamiltonian into two parts:

$$H = H_0 + \omega \quad (106)$$

where the "unperturbed" part is defined by

$$H_0(\sum_n c_n \Psi_n) = \sum_n c_n E_n \Psi_n . \quad (107)$$

In other words, the unperturbed Hamiltonian attributes to every term in our expansion the corresponding energy value of the independent-particle model. The perturbation ω is then defined by Eq. (106). Hence, the nature of our perturbation method, and its validity, may well depend on the choice we make for the method of expansion in terms of our redundant set.

For example, a particular choice leads to the same coefficients which occur in the expansion of the perturbation series Eq. (94) in eigenfunctions of the independent-particle model. The perturbation series for the energy eigenvalues also then becomes identical with that based on the independent-particle model, and to each order, the energy remains independent of k . This evidently is not a useful way of approaching the energy of translation.

It might be objected here that we had already found a translational energy of the right order of magnitude, (and for the harmonic well of the correct value) by only using the leading term of Eq. (94) in the projected function Eq. (84); this seems inconsistent with the statement that the perturbation method does not give any translational energy.

This is accounted for by the fact that we found a reasonable translational energy by taking the expectation value of the complete Hamiltonian for the function Ψ_0 , which is the projected part of the leading term of Eq. (94). If we divide the Hamiltonian into an unperturbed part and a perturbing term, we have therefore included a contribution which, in formal perturbation theory should be regarded as small of first order, and taken together with the effect of the unperturbed Hamiltonian on the first-order correction to the wave function. The first-order energy correction which appears in Eq. (105) is formed in this way, and in it the translational part (i. e., the term proportional to k^2) cancels out.

This situation gives rise to the conjecture that one may get a reasonable series of successive approximations to the translational energy if one projects on momentum k each term of the expansion Eq. (94), and then defines the S -th approximation to the energy by taking the expectation value of the complete Hamiltonian for the wave function consisting of the first S terms of the perturbation series. For the harmonic oscillator case this does indeed give the required answer in that the higher corrections to the translational energy are all zero, and the correction to the internal energy is as required. However, this is so far only a heuristic result, and has not yet been possible to put it on a proper basis, or to test its validity for the general case.

One interesting result about the set of functions Ψ_n is that this reduces to a complete set of independent functions if we restrict ourselves to those states of the independent-particle model in which one particle, say the first, remains in the ground state. These states are no longer of any particular symmetry in the particles, but this does not prevent us from expanding the required solution, which will be symmetric for bosons, or antisymmetric for fermions, in terms of them. For bosons the ground state of the independent-particle model, in which all particles are in the lowest state, belongs to this restricted set, so that we can at least start off in a physically sensible way, whereas this is not true for the fermion system.

This property of the restricted set can be proved in the following way. Consider a general function of the N coordinates, for simplicity in one dimension, which is an eigenstate of the total momentum, with eigenvalue k . We want to show that this function can be expanded in one and only one way into a series

$$F(x_1, x_2, \dots, x_N) = \sum C_{n_1 n_2 \dots n_N} \Psi_{0, n_2, n_3, \dots, n_N}(x_1, \dots, x_N).$$

Consider the Fourier transform of F :

$$F(x_1, x_2, \dots, x_N) = \int dq_1 dq_2 dq_3 \dots dq_N G(q_1, q_2, \dots, q_N) e^{i \sum_{i=1}^N q_i x_i}.$$

Since F is assumed to be a momentum eigenstate, G must be of the form

$$G(q_1, q_2, \dots, q_N) = g(q_2, q_3, \dots, q_N) \delta(k - \sum_{i=1}^N q_i).$$

Ψ_n is defined by

$$\Psi_{0, n_2, n_3, \dots, n_N} = \int e^{ikr} u_0(x_1 - r) u_{n_2}(x_2 - r) \dots u_{n_N}(x_N - r) dr$$

where the u_n are the one-particle functions in the potential well. Inserting for these their Fourier transforms, say v_n , we find after a simple transformation:

$$\Psi_n = 2\pi \int dq_2 \dots dq_N v_0(k - \sum_{i=2}^N q_i) v_{n_2}(q_2) \dots v_{n_N}(q_N) e^{i(k - \sum_{i=2}^N q_i)x_i + \sum_{i=2}^N q_i x_i}.$$

We see therefore that our expansion for F requires that

$$g(q_2, q_3, \dots, q_N) = 2\pi \sum C_{n_2 n_3 \dots n_N} v_0(k - \sum_{i=2}^N q_i) v_{n_2}(q_2) \dots v_{n_N}(q_N).$$

If we divide both sides by

$$V_0(k - \sum_i^n q_i),$$

which has no zeros, the problem is now reduced to the expansion of a known function of the $N-1$ variables $q_2 \dots q_N$ in terms of products of the v_n , which form a complete orthonormal set. This proves that the expansion is possible and that it is unique.

One may try to use this restricted set in the first-order Eq. (105), at least for a boson system. This approach is being investigated by J. Lascoux, but preliminary indications are that in the oscillator problem with harmonic forces, which we have used above as illustration, the method gives the correct translational energy to second order, but that in higher orders the answer changes, although it would presumably be right again if all orders were summed. If this is confirmed it follows that this restricted set is not a good way for making the expansion unique, its main fault being that it destroys the symmetry between the particles.

Alternative ways of making the expansion unique are now under investigation, but no concrete results are as yet available.

We conclude that the present method has not yet yielded a reliable treatment of collective motion. It seems, however, worth-while to continue the search for a satisfactory method of carrying through perturbation theory. Such a method could then immediately be applied also to the rotational problem, and would make it possible to test, and possibly to correct, the moments of inertia calculated by Yoccoz.

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HIGH-ENERGY COLLISION THEORY

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Few trends are more striking nowadays than the increase of attention being devoted to the collisions of particles accelerated to high energies. The reasons for such studies lie basically in the information they furnish about the interactions of the colliding particles, and about the reaction products they generate. Both types of information may usually be obtained more readily at high than at low energies. The study of low-energy collisions ordinarily tells us only a certain measure of the strength of an interaction. At high energies, on the other hand, the shorter wavelength of the incident particles makes them sensitive probes of the region of interaction. When the wavelengths are sufficiently short, for example, the angular distribution of elastically scattered particles becomes, in a sense, a detailed map of the region of interaction. Inelastic collisions are capable of furnishing much the same information too, and as particle energies rise, the importance of such collisions grows and their variety multiplies.

The type of problem we should like to treat, say the collision of an incident particle with a nucleus consisting of many particles, is not an easy one to formulate at any energy. But at high energies the complication of the problem as evidenced, for example, by the huge number of final states available to the system, makes the prospect of reaching exact solutions quite dim indeed. Fortunately, however, the physical conditions which hold at high energies are in a number of ways well suited to the introduction of approximation methods. The major part of these lectures will be devoted to the development of such techniques.

The approximation methods we shall describe are quite elementary in structure. They all bear a certain family resemblance to the approximations used in the diffraction theory of physical optics. That is not to say that they are too familiar, however, since the situations encountered in collision theory are usually quite different from those of optics. For example, the target particles in a nucleus are free to move about in a bound state while the obstacles of diffraction theory are always fixed. It will be necessary, therefore, to develop mathematical methods for treating the quantum mechanical problem which are of much greater generality than those of physical optics. But the mathematics required is very simple in form and furnishes insight into situations of surprising complexity.

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A great deal of the work which has thus far been done on high-energy collisions has consisted of more or less empirical studies of the so-called "optical model." This model, which has been introduced and used more often on intuitive than on mathematical grounds, represents an attempt to deal with the problem of elastic scattering alone. The optical model removes from consideration particles which undergo inelastic scatterings by pretending that they have been absorbed within the nucleus. Of course any desire to discuss this effective absorption in a quantitative way leads us back again to the question of treating inelastic processes. Any mathematically comprehensive discussion of the optical model must therefore be based on a unified treatment of elastic and inelastic transitions. One of the favorable features of the approach to be described is that it is unitary in this sense, and thereby allows a very simple insight into the origin of the optical model. The model emerges as a rather natural way of describing the particular results obtained for elastic scattering, and these enable us to give an explicit construction of the optical potential for a finite-sized nucleus. We shall use it to illustrate the way in which the optical potential depends on the fluctuations and correlations in the positions of the individual nucleons.

It may be appropriate, before beginning, to say a word about how this work developed. The work on elastic scattering was done in 1952 in connection with a problem which was of particular interest in electron diffraction theory. It produced, in effect, an extension and generalization of a method described by Molière¹ in 1947. The remainder of the work, on the treatment of nonstatic interactions accumulated slowly in the period that followed. Unfortunately the material has been published only in fragments and abstracts. Various of the unpublished results have been quoted, however, in a number of papers²⁻⁸ and so may be, to a degree, familiar. Others of the results are of more recent date and have not previously been published in any form. We shall try in these lectures to present the first systematic approach to this work, to its methods and results.

Since not everyone may be too conversant with the mathematical methods of scattering theory we shall begin with a general discussion of the simple problem of elastic scattering by a static potential. Here we shall review quite briefly some of the familiar methods of treating the problem, and shall pay particular attention to certain very useful theorems regarding the scattering amplitudes. We shall then begin the development of the high-energy approximation, and illustrate its application to a succession of problems of gradually increasing complexity. Collisions involving many-body systems will be dealt with in the last lectures.

Elastic Scattering (Formulation)

To begin with the simplest type of scattering problem, we shall assume that the incident particles are deflected by a static force field which is localized in range. The field may be represented by a potential $V(r)$. We shall take the energy of the incident particle to be

$$E = \frac{\hbar^2 k^2}{2m} \quad (1)$$

where the symbol \vec{k} will be used to represent the propagation vector of the incident wave. Our problem is to solve the Schrödinger equation

$$(\nabla^2 + k^2) \psi(\vec{r}) = \frac{2m}{\hbar^2} V(\vec{r}) \psi(\vec{r}), \quad (2)$$

subject to the boundary condition that at large distances from the region occupied by the potential the wave function has the asymptotic form

$$\psi(\vec{r}) \sim e^{ik \cdot \vec{r}} + f(\theta) \frac{e^{ikr}}{r}, \quad (3)$$

i. e., the sum of the incident plane wave and an outgoing spherical wave with scattering amplitude $f(\theta)$. We choose the incident wave to have unit density so that the incident flux is the incident velocity v . The flux scattered through solid angle $d\Omega$ is just

$$|f(\theta)|^2 \frac{1}{r^2} v r^2 d\Omega$$

so that the corresponding differential element, $d\sigma$, of the cross section is given by

$$d\sigma = \frac{\text{Flux through } d\Omega}{\text{Incident flux}} = |f(\theta)|^2 d\Omega. \quad (4)$$

The problem, as we have stated it thus far, falls into two parts. It is necessary to find functions which satisfy a partial differential equation and among these to choose the one satisfying an asymptotic boundary condition. Now for many purposes it is useful to have a more unified formulation of the problem, one which incorporates both the Schrödinger equation and its boundary condition. Such a statement may be obtained by means of an integral equation. As the first step in formulating an integral equation we define the Green's function, $G(\vec{r}, \vec{r}')$, as a solution of the inhomogeneous wave equation

$$(\nabla^2 + k^2) G(\vec{r}, \vec{r}') = \frac{2m}{\hbar^2} \delta(\vec{r} - \vec{r}'). \quad (5)$$

The similarity of this equation to the Poisson equation permits one to see that the solution has the singularity $1/|\vec{r} - \vec{r}'|$. The general solution may easily be seen to be

$$-\frac{2m}{4\pi\hbar^2} \frac{\alpha e^{ik|\vec{r}-\vec{r}'|} + \beta e^{-ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|}$$

where $\alpha+\beta=1$. We shall define $G(\vec{r}, \vec{r}')$ to be the amplitude which corresponds to the steady radiation from a coherent source at \vec{r}' . We, therefore, choose $\alpha=1$, so that our Green's function is

$$G(\vec{r}, \vec{r}') = -\frac{2m}{4\pi\hbar^2} \frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|}. \quad (6)$$

Now, it is easy to see that the expression for $\Psi(\vec{r})$ given by

$$\Psi(\vec{r}) = e^{ik\cdot\vec{r}} + \int G(\vec{r}-\vec{r}') V(\vec{r}') \Psi(\vec{r}') d\vec{r}' \quad (7)$$

satisfies the Schrödinger equation identically. To see if the asymptotic behavior is correct we expand for large $|\vec{r}'|=r'$, noting that

$$|\vec{r}-\vec{r}'| \rightarrow r - \frac{\vec{r}\cdot\vec{r}'}{r}$$

as the ratio $|\vec{r}'|/r$ approaches zero. The latter ratio is indeed small when r is large since the region of the r' integration extends only over the region where V is different from zero. Now let us define a propagation vector pointing in the direction \vec{k}_r

$$\vec{k}_r \equiv |\vec{k}| \frac{\vec{r}}{r} = k \frac{\vec{r}}{r}. \quad (8)$$

From the integral equation

$$\Psi(\vec{r}) = e^{ik\cdot\vec{r}} - \frac{2m}{4\pi\hbar^2} \int \frac{e^{ik|r-r'|}}{|\vec{r}-\vec{r}'|} V(\vec{r}') \Psi(\vec{r}') d\vec{r}' \quad (9)$$

we obtain as $r \rightarrow \infty$

$$\Psi(\vec{r}) \rightarrow e^{ik\cdot\vec{r}} - \frac{2m}{4\pi\hbar^2} \frac{e^{ikr}}{r} \int e^{-i\vec{k}_r \cdot \vec{r}'} V(\vec{r}') \Psi(\vec{r}') d\vec{r}'. \quad (10)$$

We see that this has the required asymptotic form. Furthermore, we have obtained an exact expression for the scattering amplitude.

To make the notation more explicit it will be convenient to write

$\Psi_{\vec{k}}(r)$ for the wave function which develops from an incident plane wave $e^{i\vec{k}\cdot\vec{r}}$. We may also replace the symbol $f(\theta)$ for the scattering amplitude by the more general notation $f(\vec{k}', \vec{k})$ which designates the amplitude for scattering from the direction \vec{k} to a direction \vec{k}' , where of course we have $|\vec{k}'| = |\vec{k}|$. The scattering amplitude is then given by

$$f(\vec{k}', \vec{k}) = -\frac{2m}{4\pi k^2} \int e^{-i\vec{k}' \cdot \vec{r}} V(\vec{r}) \Psi_{\vec{k}}(\vec{r}) d\vec{r}. \quad (11)$$

From this it is clear that we only need to know the wave function in the region where $V(\vec{r}) \neq 0$ in order to have an accurate evaluation of the scattering.

Identities Satisfied by the Scattering Amplitude

There are certain exact relations which the scattering amplitude obeys quite generally, and in developing approximation procedures it is wise never to let these stray far from sight. These relations have to do, first of all, with dynamical reversibility and, secondly, with conservation theorems and orthogonality relations. We shall briefly outline their derivations.

Suppose, first of all, one considers two wave functions $\Psi_{\vec{k}}(\vec{r})$ and $\Psi_{-\vec{k}'}(\vec{r})$ where $|\vec{k}| = |\vec{k}'|$, but \vec{k} and \vec{k}' are in different directions and the minus sign in the index $-\vec{k}'$ is taken only for convenience in expressing the result. It follows from the Schrödinger equation that we have the identity

$$\Psi_{-\vec{k}'} \nabla^2 \Psi_{\vec{k}} - \Psi_{\vec{k}} \nabla^2 \Psi_{-\vec{k}'} = 0. \quad (12)$$

Integrating this expression over the volume of a large sphere and using Green's Theorem, we find

$$\int_{\text{Surf of Sphere}} \left\{ \Psi_{-\vec{k}'} \frac{\partial}{\partial r} \Psi_{\vec{k}} - \Psi_{\vec{k}} \frac{\partial}{\partial r} \Psi_{-\vec{k}'} \right\} dS = 0. \quad (13)$$

Now this integration is over the surface of a very large sphere so we may use the asymptotic form of the wave function in the integrand. By making use of the propagation vector in the direction \vec{F} defined by Eq. (8) the integral relation Eq. (13) may be written as

$$\int \left\{ e^{i\vec{k}' \cdot \vec{F}} + f(\vec{k}_r, -\vec{k}') \frac{e^{i\vec{k} \cdot \vec{r}}}{r} \right\} \frac{\partial}{\partial r} \left\{ e^{i\vec{k} \cdot \vec{F}} + f(\vec{k}_r, \vec{k}) \frac{e^{i\vec{k} \cdot \vec{r}}}{r} \right\} dS - \quad (14)$$

$$-\int \left\{ e^{i\vec{k}\cdot\vec{r} + f(\vec{k}_r, \vec{k})} \frac{e^{ikr}}{r} \right\} \frac{\partial}{\partial r} \left\{ e^{-i\vec{k}'\cdot\vec{r} + f(\vec{k}_r, -\vec{k}')} \frac{e^{ikr}}{r} \right\} dS = 0.$$

The terms which contain the product of two plane waves may be seen, when summed, to furnish a vanishing integral. The terms which contain the product of two scattering amplitudes obviously cancel as well. The only remaining contributions are from terms linear in the scattering amplitude. To demonstrate the method of deriving the identity, and incidentally to introduce a procedure which will later be of use, it suffices to discuss the first of these terms linear in f , which is of the form

$$\frac{1}{r} \int f(\vec{k}_r, -\vec{k}') (\vec{k}\cdot\vec{r} - kr) e^{i(\vec{k}\cdot\vec{r} + kr)} d\Omega_r. \quad (15)$$

By writing $\mu = \cos(\hat{\vec{k}}, \hat{\vec{r}})$, and letting φ be an azimuthal angle of \vec{r} about \vec{k} , this integral may be written as

$$k \int f(\vec{k}_r, -\vec{k}') (\mu - 1) e^{ikr(\mu+1)} d\mu d\varphi.$$

This contains an integral of the general form

$$\int_{-1}^1 F(\mu) e^{ikr\mu} d\mu. \quad (16)$$

If the function F is sufficiently smooth the asymptotic form of the latter integral as $r \rightarrow \infty$ is easily evaluated. Integration by parts yields

$$\left[\frac{F(\mu) e^{ikr\mu}}{ikr} \right]_{-1}^1 - \frac{1}{ikr} \int F'(\mu) e^{ikr\mu} d\mu.$$

Further integration by parts will only give terms involving higher powers of $(kr)^{-1}$, which for a large sphere, $(kr \gg 1)$ can all be dropped. Therefore, we secure for the integral Eq. (15) the value

$$\frac{k}{ikr} \int d\varphi f(\vec{k}_r, -\vec{k}') (\mu - 1) e^{ikr(\mu+1)} \Big|_{\mu=-1}^{\mu=1}.$$

The contribution of the limit $\mu = 1$, is seen to vanish. The limit $\mu = -1$ corresponds to \vec{r} lying in the direction $-\vec{k}$. At this limit the exponential reduces to unity and the azimuthal integration degenerates to the trivial

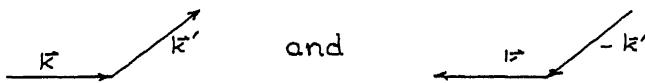
contribution of a factor 2π . The integral Eq. (15) therefore reduces asymptotically to

$$-\frac{2}{ir} \cdot 2\pi \cdot f(-\vec{k}, -\vec{k}').$$

By evaluating the other integral of Eq. (14) in the same way we obtain the relation

$$f(-\vec{k}, -\vec{k}') = f(\vec{k}', \vec{k}). \quad (17)$$

That is, the scattering amplitudes for the sequences of propagation vectors represented by the diagrams



are identically equal. The identity evidently expresses the dynamical reversibility of the system.

Now suppose we have a potential $V(\vec{r})$ which is invariant under inversion through the origin; i. e.,

$$V(\vec{r}) = V(-\vec{r}). \quad (18)$$

This is a symmetry relation which must also be reflected by a property of the scattering amplitude. In fact the physical situation remains unchanged if all momenta as well as coordinates are inverted, so that the scattering amplitude must have the symmetry

$$f(\vec{k}', \vec{k}) = f(-\vec{k}', \vec{k}). \quad (19)$$

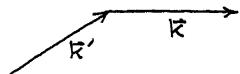
Now combining this relation with the reversibility identity, Eq. (17) we obtain

$$f(\vec{k}', \vec{k}) = f(\vec{k}, \vec{k}') \quad (20)$$

i. e., the scattering amplitude is the same for the diagram



as it is for



The symmetry Eq. (20) is of a type often invoked in arguments in kinetic theory. It might be referred to as detailed balancing symmetry. Note that no such relation need hold in general in the absence of the inversion symmetry Eq. (18).

Suppose we consider now two wave functions,

$$\Psi_k(r)$$

and a complex conjugate function

$$\Psi_{k'}^*(r),$$

and play the same game once more. As long as the potential $V(r)$ is real we have

$$\Psi_{k'}^* \nabla^2 \Psi_k - \Psi_k \nabla^2 \Psi_{k'}^* = 0. \quad (21)$$

Once again we integrate the expression over the volume of a large sphere and use Green's theorem to introduce an integration over the surface of the sphere. A number of the integrals cancel as in Eq. (14) and two terms linear in the scattering amplitude again survive. In addition there is a term quadratic in the scattering amplitudes which also survives because of the operation of complex conjugation which has been introduced in Eq. (21). When the integrals are evaluated asymptotically just as they were before we are left with the identity⁹

$$\frac{1}{2i} \{ f(k', k) - f^*(k, k') \} = \frac{k}{4\pi} \int f''(k_r, k) f(k_r, k) d\Omega_r. \quad (22)$$

For the case $k' = k$ this relation reduces to a particularly simple form

$$\begin{aligned} \text{Im } f(k, k) &= \frac{k}{4\pi} \int |f(k_r, k)|^2 d\Omega_r \\ &= \frac{k}{4\pi} \sigma_{\text{Scatt.}}, \end{aligned} \quad (23)$$

where $\sigma_{\text{scatt.}}$ is the total scattering cross section. This identity, sometimes referred to as the "optical theorem" is easily seen to represent no more than the requirement of particle conservation. Indeed the quantum mechanical particle current for a state $\Psi_k(\vec{r})$ is

$$\vec{j} = \frac{\hbar}{2im} \{ \Psi_k^* \nabla \Psi_k - \Psi_k \nabla \Psi_k^* \}, \quad (24)$$

so that for $\vec{k} = \vec{k}'$, Eq. (21) represents simply the conservation condition for a stationary state,

$$\nabla \cdot \vec{j} = 0. \quad (25)$$

The particular form of the identity, Eq. (23), may be understood as follows: The flux of scattered particles travelling off in spherical waves is proportional to $\sigma_{\text{scatt.}}$. Such particles can have their origin only in a decrease of the strength of the incident plane wave. This decrease is accomplished by means of a destructive interference between the plane wave and the scattered wave which takes place near the forward direction. Eq. (23) represents the balancing of this destructive interference against the outward flux.

Some further light is shed on the identity Eq. (22) particularly for the case $\vec{k}' \neq \vec{k}$ by brief reference to the time dependent formulation of scattering theory. It is well known that the operator which, applied to the initial state of a particle, yields its final state, must always be unitary. The unitarity condition, in the case of a scattering problem, may be shown to correspond precisely to the identity Eq. (22). Such unitarity conditions not only play the role of enforcing particle conservation, but enforce the preservation of orthogonality relations as well.

For reasons that we shall later discuss at length it is often convenient to deal with the mathematical abstraction of a potential $V(\vec{r})$ which takes on complex values. We shall try to show that this concept is a very natural one to use in describing interactions in systems which produce inelastic scattering in addition to elastic scattering. For the present, however, our interest is only to see how the occurrence of a complex potential as opposed to a real one influences the identities discussed earlier.

The proof of the reversibility theorem, Eq. (17), is, in fact, in no way altered by the presence of a complex potential, i.e., we still have

$$f(-\vec{k}, -\vec{k}') = f(\vec{k}', \vec{k}).$$

The derivation of the unitarity theorem, on the other hand, involved the operation of complex conjugation and, as a consequence, is appreciably altered by giving the potential a nonvanishing imaginary part. Eq. (21) must be replaced by the relation

$$\Psi_{k'}^* \nabla^2 \Psi_k - \Psi_k \nabla^2 \Psi_{k'}^* = \frac{4m}{\hbar^2} (\text{Im } V(\vec{r})) \Psi_{k'}^* \Psi_k , \quad (26)$$

which by the same methods we used earlier leads to the identity:

$$\begin{aligned} \frac{1}{2i} \{ f(k', k) - f^*(k, k') \} &= \frac{k}{4\pi} \int f''(k_r, k') f(k_r, k) d\Omega_r \\ &\quad - \frac{m}{2\pi\hbar^2} \int (\text{Im } V(\vec{r})) \Psi_{k'}^* \Psi_k d\vec{r}. \end{aligned} \quad (27)$$

Again to secure an interpretation of this identity for the case $\vec{k} = \vec{k}'$ it is instructive to consider the divergence of the particle current vector. In the presence of a complex potential the current is no longer divergenceless. Instead, we have

$$\nabla \cdot \vec{j} = \frac{2}{\hbar} (\text{Im } V) |\Psi_k|^2 \quad (28)$$

so that, for example, at a point at which $\text{Im } V < 0$, particles are being absorbed at a rate proportional to their local density. Since the incident beam has unit density we may introduce an absorption cross section σ_{abs} . for the potential by saying that the total rate at which particles are disappearing is $v\sigma_{\text{abs}}$:

$$v\sigma_{\text{abs.}} = - \int \nabla \cdot \vec{j} d\vec{r} = - \frac{2}{\hbar} \int (\text{Im } V) |\Psi_k|^2 d\vec{r}. \quad (29)$$

For $\vec{k} = \vec{k}'$, the identity Eq. (27) may now be written in the form of a generalized "optical theorem,"

$$\begin{aligned} \text{Im } f(k, k) &= \frac{k}{4\pi} \sigma_{\text{scatt.}} + \frac{mv}{4\pi} \sigma_{\text{abs.}} \\ &= \frac{k}{4\pi} (\sigma_{\text{scatt.}} + \sigma_{\text{abs.}}) = \frac{k}{4\pi} \sigma_{\text{tot.}} \end{aligned} \quad (30)$$

This simply states that the attenuation of the incident beam by interference is accounted for by the particles absorbed in addition to those scattered. In particular this relation shows clearly that absorption is always accompanied by scattering, at least in the forward direction, i. e., $\sigma_{\text{abs.}} > 0$ implies

$$\text{Im } f(k, k) > 0,$$

from which it follows that

$$|f(\vec{k}, \vec{k})|^2 > 0.$$

Partial Wave Expansion

The most familiar approach to scattering problems is based on an expansion of the unknown wave function in spherical harmonics. We shall only give the briefest of outlines of this method in order that it may be compared with procedures to be developed later. Further details are widely available in the literature.

When a scattering potential has axial symmetry about the propagation direction of an incident wave, the wave function may be expanded in the series

$$\Psi_k(r) = \sum_l g_l(kr) P_l(\mu) \quad (31)$$

where $P_l(\mu)$ is the l -th Legendre Polynomial with argument $\mu = \cos(\hat{k} \cdot \hat{r})$. This expansion is particularly convenient for central potentials since the conservation of orbital angular momentum causes the Schrödinger equation to reduce to a succession of uncoupled ordinary differential equations for the radial functions g_l .

It is easily shown that at large distances from the scattering potential the functions $g_l(kr)$ are simple superpositions of incoming and outgoing spherical waves. The asymptotic forms of these functions may be written as

$$g_l(kr) \sim -\frac{2l+1}{2ikr} \left\{ (-1)^l e^{-ikr} - C_l e^{ikr} \right\}, \quad (32)$$

where the coefficients have been chosen so that $C_0 = 1$ when the scattering potential vanishes, and

$$\Psi_k(r) = e^{ik\vec{k} \cdot \vec{r}}.$$

The deviations of the coefficients C_l from unity furnish a description of the effect of the potential on the outgoing wave, i. e., the scattering.

The asymptotic form of the entire wave function is evidently given by

$$\Psi_k(r) - e^{ik\vec{k} \cdot \vec{r}} \sim \frac{e^{ikr}}{2ikr} \sum_l (2l+1)(C_l - 1) P_l(\mu),$$

$$\frac{Va}{\hbar v} \ll 1 . \quad (40)$$

Unfortunately, this condition is virtually never fulfilled in nuclear collisions. The problems to which it may safely be applied are usually those involving the electromagnetic interactions of fast charged particles with other particles of charge, say,

$$Z \lesssim 10 .$$

Another approximation, the W. K. B. method, corresponds to the classical limit of quantum mechanics. We assume the potential to be smooth enough that the distance over which it changes its value appreciably is large compared to the wavelength, i. e., $ka \gg 1$. Now if the kinetic energy of the incident particles is large enough, the scattering will be heavily concentrated at small angles. To see this, we will suppose that Θ is a typical scattering angle. Then as an order of magnitude approximation we may write

$$\Theta \sim \frac{\Delta p}{p} ,$$

where p is the original momentum and Δp is the change of momentum. Hence Θ is given roughly by

$$\Theta \sim \frac{\int F dt}{p} ,$$

where F is the force acting on the particle. The magnitude of the force is

$$F \sim \frac{V}{a} .$$

Now the time taken by the particle in crossing the potential is approximately

$$t = \int dt \sim \frac{a}{v}$$

so that

$$\Theta \sim \frac{V}{pv} \sim \frac{V}{E} . \quad (41)$$

which, shows as one might expect, that at sufficiently high energies the

scattering takes place predominantly through small angles.

Now the problem, of course, is not a classical but a quantum mechanical one. When a particle is known to pass through a region of dimension a the transverse component of its momentum is rendered uncertain to the extent

$$\delta p \sim \frac{\hbar}{a} .$$

The angle through which it is scattered is therefore rendered uncertain to the extent

$$\delta\theta \sim \frac{\hbar}{ap} .$$

The situation is a semi-classical one only in the limit in which particle trajectories become uniquely defined, in particular in the limit in which the uncertainty in the scattering angle becomes much smaller than the scattering angle itself

$$\frac{\theta}{\delta\theta} \sim \frac{V}{E} \frac{ap}{\hbar} \gg 1$$

or

$$\frac{Va}{\hbar v} \gg 1 . \quad (42)$$

Thus the region of applicability of the W. K. B. method does not overlap that of the Born approximation at all. We have in fact a considerable gap of values of

$$\frac{Va}{\hbar v}$$

to which neither method applies. (A unique exception to this statement must be made, however, for the case of one-dimensional problems. In these the scattering angle is either 0 or π and the argument used to derive Eq. (42) no longer applies. In one dimension the W. K. B. approximation may be accurate for arbitrary values of

$$\frac{Va}{\hbar v} .)$$

Since a certain ambiguity of terminology regarding the W. K. B. method is prevalent, it may be of help to spend a moment considering the approximation explicitly. We write the wave function in the form

$$\Psi_k(r) = e^{\frac{i}{\hbar} S^{(0)} + S^{(1)}} \quad (43)$$

where $S^{(0)}$ and $S^{(1)}$ are functions to be determined. We define the magnitude of the momentum, as it depends on position, by

$$p^2(r) = 2m[E - V(r)]. \quad (44)$$

We then substitute these into the Schroedinger equation and secure

$$-(\nabla(S^{(0)} - i\hbar S^{(1)}))^2 + i\hbar \nabla^2(S^{(0)} - i\hbar S^{(1)}) + p^2(r) = 0.$$

Now, we consider the exponent of the expression above for $\Psi_k(r)$ as an expansion in powers of \hbar , so that this last equation gives us the two equations

$$(\nabla S^{(0)})^2 = p^2(r) \quad (45)$$

and

$$\nabla S^{(0)} \cdot \nabla S^{(1)} + \nabla^2 S^{(0)} = 0. \quad (46)$$

The first of these is just the classical Hamilton-Jacobi equation whose solution may be expressed as the action integral

$$S^{(0)}(r) = \int_{\text{dynamical path}}^r p(r') dr'. \quad (47)$$

Note that, written in the form

$$\nabla S^{(0)} = \vec{p}(r),$$

this equation states that the possible trajectories of the particle are normal to the surfaces of constant $S^{(0)}$.

By using the integrating factor

$$e^{2S^{(1)}}$$

the second equation yields

$$\nabla \cdot (\nabla S^{(0)} e^{2S^{(1)}}) = 0$$

or

$$\nabla \cdot (\bar{p}(r) |\psi|^2) = 0 \quad (48)$$

which, on interpreting

$$\frac{1}{m} \bar{p}(r)$$

as the velocity field and

$$|\psi|^2$$

as the density of particles, is seen to be just the hydrodynamical equation of continuity. Now suppose a beam of particles is projected toward a scattering center. The density of particles, according to the equation, is at all points the density present if the particles simply move along their classical trajectories. Hence cross sections, for example, computed by the W. K. B. method will be precisely the same as those computed classically. (An exception arises only if the potential is sufficiently complicated that more than one classical trajectory can lead to the point of observation. In that case, Eq. (43) must be replaced by a sum of similarly constructed terms, one for each path, and non-classical interference effects arise.)

A number of authors have applied the name of the W. K. B. approximation to a rather different procedure based on the partial wave expansion. They integrate the radial equations to find the individual phase shifts by a one-dimensional W. K. B. method. The region of applicability of this procedure is altogether different from that of the one described above, although, of course, the two overlap at the classical extreme. It is questionable whether such an alternative procedure should be referred to simply as the W. K. B. approximation since its use of exact angular eigenfunctions leads to such different mathematical properties. This approximation is, in fact, related to one which we shall describe presently.

The High-Energy Approximation in One Dimension

We shall now begin the development of an approximation which is better suited to many of the purposes of high-energy studies than any of the methods mentioned earlier. While the method to be discussed is not without limitations of its own, these, as we shall see, allow one to estimate correctly the intensity of a predominant part of the scattering.

To begin the development at the simplest possible point, and one that will later prove quite useful, we shall consider a one-dimensional scattering problem. Of course it is necessary to bear in mind a very special property of scattering problems in one dimension. The scattering process can take place in only two directions, either preserving the sense of motion of the particle or sending it directly backward. There are no compromises. While this makes the problem a trifle unrealistic, it has the advantage of making it mathematically more transparent.

The Schrödinger equation in one dimension is

$$\left(\frac{d^2}{dx^2} + k^2 \right) \psi(x) = \frac{2m}{\hbar^2} V(x) \psi(x). \quad (49)$$

Now we shall assume that the energy of the incident particle greatly exceeds the magnitude of the potential $V(x)$, and is also large enough that the particle wavelength is much smaller than the potential width a

$$\frac{V}{E} \ll 1, \quad ka \gg 1. \quad (50)$$

(In order of magnitude relations such as this the symbol V is to be interpreted as a measure of the absolute magnitude of the potential.) Under these conditions we are justified in assuming that back-scattering will be very weak, that the wave function of the particle may to a good approximation be written in the form

$$\psi(x) = e^{ikx} \varphi(x), \quad (51)$$

where $\varphi(x)$ is a function which varies slowly over a particle wavelength. Substituting into the Schrödinger equation, we secure

$$(2ik \frac{d}{dx} + \frac{d^2}{dx^2}) \varphi(x) = \frac{2m}{\hbar^2} V(x) \varphi(x). \quad (52)$$

Now our approximation consists in dropping the

$$\frac{d^2}{dx^2}$$

term since we assume φ varies slowly in a wavelength. In that case the equation reduces to

$$\frac{d\varphi}{dx} = - \frac{i}{\hbar v} V(x) \varphi(x). \quad (53)$$

Now if Eq. (51) is to reduce to the incident plane wave at $x = -\infty$ (i. e., back-scattering is neglected) we require as a boundary condition $\varphi(-\infty) = 1$. Thus we secure

$$\varphi(x) = e^{-\frac{i}{\hbar v} \int_{-\infty}^x V(x') dx'} \quad (54)$$

and

$$\psi(x) = e^{ikx - \frac{i}{\hbar v} \int_x^\infty V(x') dx'} \quad (55)$$

Note that if the exponential, $\varphi(x)$, were expanded in a power series, the successive terms would represent those of the Born approximation series. In this way, we may verify directly that the expansion parameter of the series is

$$\sqrt{a/\hbar v}.$$

The approximation we have just described may be derived in another way which is also fairly instructive. Here we begin with the one-dimensional version of the integral equation for scattering

$$\psi(x) = e^{ikx} + \int G(x-x') V(x') \psi(x') dx'. \quad (56)$$

The one-dimensional Green's function we require may be expressed as

$$G(x-x') = -\frac{m}{\pi \hbar^2} \int_{-\infty}^{\infty} \frac{e^{i\lambda(x-x')}}{\lambda^2 - k^2 - i\epsilon} d\lambda, \quad (57)$$

where the outgoing wave boundary condition for G requires that we take the limit of this expression as $\epsilon \rightarrow 0$ through positive values. The result is simply

$$G(x-x') = -\frac{i}{\hbar v} e^{ik|x-x'|}. \quad (58)$$

We again express $\psi(x)$ in the form

$$\psi(x) = e^{ikx} \varphi(x),$$

so that the integral equation for φ becomes

$$\varphi(x) = 1 - \frac{i}{\hbar v} \int_{-\infty}^{\infty} e^{ik|x-x'| - ik(x-x')} V(x') \varphi(x') dx' \quad (59)$$

$$= 1 - \frac{i}{\hbar v} \int_{-\infty}^x V(x') \varphi(x') dx' - \frac{i}{\hbar v} \int_x^{\infty} e^{2ik(x-x')} V(x') \varphi(x') dx'. \quad (60)$$

When the two regions of integration $x' < x$ and $x' > x$ are separated, their integrands are seen to vary in altogether different ways. Now if the functions $V(x)$ and φ both vary slowly in a particle wavelength, the rapidly oscillating exponential in the second integrand may be expected to reduce its contribution considerably in magnitude. As a first approximation, therefore, we shall neglect the integral over the region $x' > x$. It is clear from the form of this integral that we are thereby neglecting back-scattering. The integral equation which remains is simply

$$\varphi(x) = 1 - \frac{i}{\hbar v} \int_{-\infty}^x V(x') \varphi(x') dx', \quad (61)$$

which may be solved trivially by differentiating, so that we are again led to the differential equation

$$\frac{d\varphi(x)}{dx} = - \frac{i}{\hbar v} V(x) \varphi(x)$$

with the boundary condition

$$\varphi(-\infty) = 1,$$

and the solution

$$\varphi(x) = e^{ikx - \frac{i}{\hbar v} \int_{-\infty}^x V(x') dx'}. \quad (55)$$

The restrictions underlying this result may be clearly seen from the above. We require that both $V(x)$ and $\varphi(x)$ vary slowly within a wavelength. The first of these conditions is $ka \gg 1$ where a is the width of the potential. The second condition, is indicated by the form derived for $\varphi(x)$. We evidently require

$$k \gg \frac{V}{\hbar v}$$

or

$$| \gg V/E .$$

These are the conditions, Eq. (50), stated earlier.

It should be noted particularly that even though the assumptions

$$ka \gg 1$$

and

$$V/E \ll 1$$

are required above, no restriction has been placed on the product of these two quantities. Now their product is

$$ka \cdot \frac{V}{E} = 2 \frac{Va}{\hbar v} , \quad (62)$$

so we see that the present approximation, in contrast with those discussed earlier, remains valid for arbitrary values of the important parameter

$$Va/\hbar v .$$

Before discussing higher approximations we might point out that the form Eq. (55) for the wave function may also be reached by means of the W. K. B. method. One has only to expand the familiar W. K. B. approximation to a one-dimensional wave function in power of V . But, unfortunately this is a shortcut confined to one dimensional problems. The one-dimensional W. K. B. approximation, as we have noted earlier, is unusual in that it need not require

$$Va/\hbar v \gg 1 ,$$

and may in this case overlap the present approximation. In two or more dimensions, however, this overlap disappears. The direct generalization of the method we are discussing yields results which only coincide with those of the W. K. B. approximation in the limit

$$Va/\hbar v \rightarrow \infty .$$

In order to improve the accuracy of the approximation, explicit account must be taken of the back-scattered wave. For this purpose, we write the wave function as,

$$\psi(x) = e^{ikx} \varphi_+(x) + e^{-ikx} \varphi_-(x) . \quad (63)$$

a form which possesses sufficient generality that the functions φ_+ and φ_- both need only vary slowly within a wavelength. There are various ways of writing equations for the determination of φ_{\pm} . One method is to construct a pair of coupled integral equations equivalent to Eq. (56). A much simpler procedure, however, is to write a pair of coupled first order differential equations equivalent to the Schrödinger equation,

$$\frac{d\varphi_+(x)}{dx} = -\frac{i}{\hbar v} V(x) \varphi_+(x) - \frac{i}{\hbar v} e^{-2ikx} V(x) \varphi_-(x) \quad (64)$$

$$\frac{d\varphi_-(x)}{dx} = +\frac{i}{\hbar v} V(x) \varphi_-(x) + \frac{i}{\hbar v} e^{2ikx} V(x) \varphi_+(x) . \quad (65)$$

The second order equation for $\psi(x)$ to which these reduce is precisely the wave Eq. (49). The boundary conditions on φ_{\pm} may be seen from the form of the expression Eq. (63) for $\psi(x)$. Since a plane wave is incident from $-\infty$ we choose

$$\varphi_+(-\infty) = 1 ,$$

and since there can be no back-scattered wave present at $+\infty$, we choose

$$\varphi_- (\infty) = 0 .$$

The amplitude for back-scattering may then be defined to be

$$\varphi_-(-\infty) .$$

If back-scattering is neglected, i.e., φ_- is assumed to vanish as a first approximation, Eq. (64) reduces to the form, Eq. (53), considered earlier. Since the back-scattering is characteristically quite weak under the conditions Eq. (50), an expansion begun in this way must converge rapidly. We may therefore use an iteration procedure in the solution, writing φ_{\pm} in the form

$$\begin{aligned} \varphi_+ &= \varphi_+^{(0)} + \varphi_+^{(1)} + \dots \\ \varphi_- &= \varphi_-^{(1)} + \varphi_-^{(2)} + \dots \end{aligned} \quad (66)$$

where the numerical indices indicate the number of iterations required to reach that particular term, i.e., we begin with

$$\varphi_+^{(0)}(x)$$

given by Eq. (54), substitute this in Eq. (65), solve for

$$\underline{\varphi}^{(1)}(x)$$

then use this in Eq. (64), and so on.

The first approximation to the back-scattering amplitude is found to be

$$\varphi^{(1)}(\infty) = -\frac{i}{\hbar v} \int_{-\infty}^{\infty} e^{2ikx} V(x) e^{-\frac{2i}{\hbar v} \int_x^{\infty} V(x') dx'} dx . \quad (67)$$

If the potential V is as smooth as assumed, and

$$\frac{V}{E} \ll 1 ,$$

this is indeed quite small. The higher terms in the expansions of the forward and backward amplitudes introduce corrections which are of order V/E and $1/ka$ relative to Eq. (54) and Eq. (67).

The High-Energy Approximation in Three Dimensions

Three-dimensional problems are, of course, the ones that interest us most. We shall try to develop a means of treating these that stays as close as possible in spirit to the one-dimensional procedure just described. The integral equation in three dimensions is

$$\Psi_k(\vec{r}) = e^{ik\cdot\vec{r}} - \frac{2m}{4\pi\hbar^2} \int \frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|} V(\vec{r}') \Psi_k(\vec{r}') d\vec{r}' .$$

Here again we separate the wave function into the product of the incident plane wave and a factor which modulates it

$$\Psi(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} \varphi(\vec{r}) \quad (68)$$

and obtain the equation for φ

$$\varphi(\vec{r}) = 1 - \frac{2m}{4\pi\hbar^2} \int \frac{e^{ik|\vec{r}-\vec{r}'|-i\vec{k}\cdot(\vec{r}-\vec{r}')}}{|\vec{r}-\vec{r}'|} V(\vec{r}') \varphi(\vec{r}') d\vec{r}' . \quad (69)$$

We now define a new position variable \vec{r}'' by

$$\vec{r}'' = \vec{r} - \vec{r}' ,$$

so that the above equation becomes

$$\varphi(\vec{r}) = 1 - \frac{2m}{4\pi\hbar^2} \int \frac{e^{i(kr'' - \vec{k}\cdot\vec{r}'')}}{r''} V(r-r'') \rho(r-r'') d\vec{r}'' . \quad (70)$$

We also assume, as before, that the product $V\rho$ varies slowly within a particle wavelength, $1/k$, so that negligibly small contributions to the integral on the right come from regions in which the exponential oscillates rapidly. If we consider points \vec{r}'' which lie within the volume occupied by the potential, the largest contributions to the integral will come from values of \vec{r}'' lying close in direction to \vec{k} , since for these the exponential is nearly stationary. The quantitative expression of this approximation is obtained by carrying out the angular integration over \vec{r}'' by means of the asymptotic method discussed earlier in connection with the expression Eq. (16). The differential element $d\vec{r}''$ may be written as

$$d\vec{r}'' = r''^2 dr'' d\mu d\phi ,$$

where

$$\mu = \cos(\hat{\vec{k}}, \hat{\vec{r}}')$$

and ϕ is an azimuthal angle.

Now, let us suppose, to be specific, that the product $V\rho$ varies appreciably only within a distance d . We shall discuss this distance later, but for the time being we shall assume it to be much larger than $\lambda = 1/k$. If the integration over μ is carried out by parts and only the leading term retained, we secure

$$\varphi(\vec{r}) = 1 + \frac{2m}{4\pi\hbar^2} \int r''^2 dr'' d\phi \left[\frac{e^{ikr''(1-\mu)}}{ikr''} V(r-r'') \rho(r-r'') \right]_{\mu=-1}^{+\infty} + O(\frac{1}{kd})$$

The terms neglected by the asymptotic approximation are as indicated, of relative order $1/kd$. Now the limit $\mu=-1$ corresponds to \vec{r}'' anti-parallel to \vec{k} . Since the exponential varies rapidly in this case the contributions of the $\mu=-1$ term is of order $1/kd$ and is therefore negligibly small. We are thus left simply with the term corresponding to \vec{r}'' parallel to \vec{k} ,

$$\varphi(\vec{r}) = 1 - \frac{i}{\hbar\nu} \int_0^\infty V(r-r'') \rho(r-r'') \Big|_{r'' \parallel \vec{k}} dr'' \quad (71)$$

The appearance of this equation is somewhat simpler in cartesian coordinates. We choose the positive z axis to lie in the direction of propagation \vec{k} , thus obtaining

$$\varphi(x, y, z) = 1 - \frac{i}{\hbar v} \int_{-\infty}^z V(x, y, z') \varphi(x, y, z') dz' . \quad (72)$$

This equation is seen to be of precisely the form encountered in the one-dimensional problem. In fact the present approximation treats the three-dimensional problem as a bundle of parallel one-dimensional ones. The solution to Eq. (72) is immediately seen to be

$$\varphi(x, y, z) = e^{-\frac{i}{\hbar v} \int_{-\infty}^z V(x, y, z') dz'} \quad (73)$$

so that the approximate wave function is

$$\psi(x, y, z) = e^{ikz - \frac{i}{\hbar v} \int_{-\infty}^z V(x, y, z') dz'} . \quad (74)$$

Now this expression is missing a good many of the things one looks for in a three-dimensional wave function, e. g., a spherical outgoing wave, but we must remember that the arguments from which it is derived are only intended to hold within the volume occupied by the potential. The expression Eq. (74) therefore need not represent the wave function well elsewhere. Fortunately, as we pointed out in connection with Eq. (11), it is only necessary to know the wave function within the volume of the potential in order to find the scattering amplitude.

Before evaluating the scattering amplitude, it may be of interest to indicate another way of phrasing the approximation just described.¹⁰ For this purpose we introduce the Fourier integral representation of the three dimensional Green's function

$$G(\vec{r}-\vec{r}') = -\frac{2m}{(2\pi)^3 \hbar^2} \int_{\epsilon \rightarrow +0} \frac{e^{i\vec{\lambda} \cdot (\vec{r}-\vec{r}')}}{\lambda^2 - k^2 - i\epsilon} d\vec{\lambda} . \quad (75)$$

Now the situation we are attempting to describe, in which we characteristically require

$$ka \gg 1$$

and

$$V/E \ll 1$$

is one in which, as we have noted earlier, the scattering is heavily concentrated at small angles. It is, in fact, very unlikely that in traversing the potential the particle will be deflected greatly from its initial direction \vec{k} . If we were to treat the problem in momentum space, we could secure an approximation to the wave function by expanding its momentum dependence about the value \vec{k} . An equivalent procedure may be based on the expansion of the momentum space dependence of the Green's function about the point \vec{k} , i. e., in the problem in question only values of \vec{x} near \vec{k} in the integrand of Eq. (75) will play roles of any importance. We may therefore write

$$\vec{x} = \vec{k} + \vec{n}$$

in the integrand, retaining the first power of n and expanding higher powers. When this reduced form of the Green's function is substituted into the usual three-dimensional integral equation, the equation simplifies once more to the form (72).

This second form of the approximation, although a bit more cumbersome than the first, brings out a certain limitation of the approach more clearly. The approximate wave function, Eq. (74), is only adequate for the treatment of small-angle scattering. It does not contain, in general, a correct estimate of the Fourier amplitudes corresponding to large momentum transfer. In fact, quantitatively, the limitation on scattering angles may be shown to be given roughly by

$$\Theta^2 kd \ll 1 \quad (76)$$

where d is again the distance within which $V\varphi$ varies. Although this limitation is a strong one, we shall see that it is nevertheless consistent with an accurate representation of the total scattered intensity.

In order to evaluate the scattering amplitude, it will be convenient to define certain coordinate vectors. Let \hat{R} be a unit vector,

$$|\hat{R}| = 1,$$

pointing in the incident propagation direction \vec{k} which, as before, will also be taken to determine the positive z -axis. Then any position vector \vec{r} may be resolved into two components.

$$\vec{r} = \vec{\sigma} + \hat{R} z, \quad (77)$$

where $\vec{\sigma}$ is a vector lying in a plane perpendicular to \vec{k} (see Fig. 1). With this notation, $\psi(\vec{r})$ as given by Eq. (74) may be written

$$\psi(\vec{r}) = e^{i\vec{k}\cdot\vec{r} - \frac{i}{\hbar v} \int_{-\infty}^z V(\vec{\sigma} + \hat{R} z') dz'} . \quad (78)$$

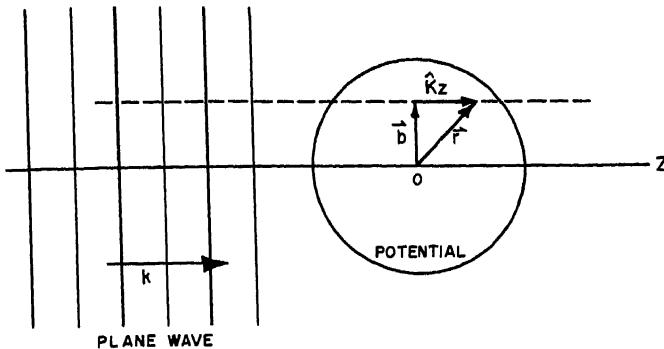


Fig. 1

Here, if the potential is centered at the origin, the distance $b = |\vec{b}|$ evidently has the interpretation of an impact parameter.

Now, substituting the above wave function into the expression Eq. (11) for the scattering amplitude, we secure

$$f(\vec{k}', \vec{k}) = -\frac{2m}{4\pi\hbar^2} \int e^{ik'\cdot\vec{r}} V(\vec{r}) e^{ik\cdot\vec{r} - \frac{i}{\hbar v} \int_{-\infty}^z V(b + \vec{R}z) dz'} d\vec{z} d^{(2)}b$$

where $d^{(2)}b$ denotes integration over the plane of impact vectors. This can be written as

$$f(\vec{k}', \vec{k}) = -\frac{2m}{4\pi\hbar^2} \int e^{i(\vec{k}-\vec{k}')\cdot(b+\vec{R}z)} V(b+\vec{R}z) e^{-\frac{i}{\hbar v} \int_{-\infty}^z V(b+\vec{R}z) dz'} d\vec{z} d^{(2)}b. \quad (79)$$

Now, energy conservation requires $|\vec{k}'| = |\vec{k}|$ so that for small scattering angles the vector $\vec{k}-\vec{k}'$ is nearly perpendicular to \vec{k} . In fact, the error of approximating the exponential

$$\exp[i(\vec{k}-\vec{k}')\cdot\hat{k}_z]$$

by unity is only of order

$$(1 - \cos\theta)kd \sim \theta^2 kd,$$

where θ is the scattering angle and d the distance within which $V\varphi$ varies appreciably. As we have noted earlier, the limitation

$$\Theta^2 k d \ll 1$$

already underlies the wave function used so that this approximation introduces no further restriction. With this simplification, the z -integration is simply that of an exact differential and leads to

$$f(\vec{k}', \vec{k}) = \frac{k}{2\pi i} \int e^{i(\vec{k}-\vec{k}') \cdot \vec{b}} \left\{ e^{-\frac{i}{\hbar v} \int_{-\infty}^{\infty} V(b + \hat{K}z) dz'} - 1 \right\} d^{(3)} b . \quad (80)$$

This is the basic result for elastic scattering. It may be thought of as corresponding to a picture in which each portion of the incident wave passes through the potential along a straight-line path and suffers a shift of phase characteristic of that path.

For potentials with azimuthal symmetry we may carry the integration one step further by noting that

$$\frac{1}{2\pi} \int_0^{2\pi} e^{i\lambda \cos \phi} d\phi = J_0(\lambda) \quad (81)$$

where $J_0(\lambda)$ is the zeroth order Bessel function. So, using the small-angle expression

$$(\vec{k} - \vec{k}') \cdot \vec{b} = kb\theta \cos\phi$$

we obtain for axially symmetric potentials

$$f(\theta) = \frac{k}{l} \int J_0(kb\theta) \{ e^{i\chi(b)} - 1 \} b db , \quad (82)$$

where

$$\chi(b) = -\frac{1}{\hbar v} \int_{-\infty}^{\infty} V(b + \hat{K}z) dz . \quad (83)$$

While the methods used in carrying out the above approximation may not be too familiar, results of the form indicated have a long and venerable history in the study of physical optics. The expression Eq. (82) may be recognized as the type of formula one would use to discuss diffraction by a transparent obstacle. The traditional way, for example, of

finding the diffraction pattern formed by a thin lens would proceed as follows: one would assume that the wave is given within and near the lens by a modulated plane wave such as Eq. (76). This expression would be used to evaluate the wave on an imaginary screen placed immediately behind the lens and it would then be possible to evaluate the wave in the half-space behind the screen by the use of Green's theorem.

Precisely this method of deriving Eq. (82) as a quantum mechanical result was introduced by Molière¹ in 1947. The classic derivation, however, using the imaginary screen, becomes rather awkward in the presence of long range or slowly decreasing potentials. It is furthermore a bit less easy to generalize in other directions than the procedure we have outlined.

We shall now take a closer look at the accuracy and the limitations of the approximations we have made. We have assumed that if $V\varphi$ varies in a distance d , we may consistently neglect terms of relative order $1/kd$. Now what is the distance d ? The potential varies in a distance a , and according to Eq. (73), $\varphi(F)$ varies appreciably in a distance $\hbar v/V$. Evidently the distance d is, in order of magnitude, the smaller of these, i.e., for

$$\frac{\sqrt{a}}{\hbar v} < 1$$

we have

$$d \sim a$$

and for

$$\frac{\sqrt{a}}{\hbar v} > 1$$

we have

$$d \sim \hbar v/V.$$

In either of these cases we evidently require, as before, both the conditions

$$ka \gg 1 \quad \text{and} \quad E/V \ll 1 \quad (84)$$

To find the angular range of the approximation we remember the limitation

$$\Theta^2 kd \ll 1.$$

For the case

$$\frac{Va}{\hbar v} < 1$$

this means the approximation is only consistent for angles smaller than an angle of order of magnitude

$$1/\sqrt{ka};$$

hence

$$\theta < O\left(\frac{1}{\sqrt{ka}}\right) \quad \text{for} \quad \left(\frac{Va}{\hbar v} < 1\right). \quad (85)$$

For

$$\frac{Va}{\hbar v} > 1$$

on the other hand, the limitation is

$$\theta < O\left(\frac{\sqrt{V}}{E}\right), \quad \left(\frac{Va}{\hbar v} > 1\right). \quad (86)$$

Both of these, according to our assumptions Eq. (84), are indeed small angles. However, it is quite important to note that nearly all of the scattered intensity is concentrated, in both cases, at angles which are much smaller still, i. e., for

$$\frac{Va}{\hbar v} < 1$$

it is clear from the Born approximation that an average angle of scattering is

$$\langle \theta \rangle \sim \frac{1}{ka}, \quad \left(\frac{Va}{\hbar v} < 1\right), \quad (87)$$

while for

$$\frac{Va}{\hbar v} > 1$$

the argument given in connection with the W. K. B. method (see relation (41)) shows

$$\langle \theta \rangle \sim \frac{\sqrt{V}}{E}, \quad \left(\frac{Va}{\hbar v} > 1\right). \quad (88)$$

In both extremes the typical scattering angles are well within the angular range of the approximation. These inequalities have a most important consequence. They allow the approximation to furnish satisfactory esti-

mates of total cross sections in spite of its limited angular range. We shall presently demonstrate the self-consistency of this feature of the high-energy approximation by showing that its expression for the small-angle scattering amplitude obeys the optical theorem.

While the approximation we have been discussing is limited in application to small-angle scattering, there is a simple way in which its angular range may be increased somewhat. This corresponds to removing an artificial asymmetry which we have allowed to creep into the derivation of the approximate expression for the scattering amplitude. In the foregoing derivation the incident propagation vector \vec{k} played a unique role in the determination of the approximate wave function while the final propagation vector \vec{k}' appeared only in a plane wave factor. Now the scattering amplitude always has a certain symmetry under the interchange of these two vectors. The most general such symmetry is that under velocity reversal which we noted earlier, in Eq. (17). It is a simple matter to find a formulation of the scattering amplitude, which has the advantage over Eq. (11) of being more manifestly symmetric under velocity reversal. We shall not go into the details of the altered derivation since, to a large degree, they resemble those we have just discussed. Suffice it to say, that the only change required in the result Eq. (80) for the scattering amplitude is a slight shift in the direction of the unit vector \vec{R} . Instead of choosing \vec{R} to lie in the incident direction, we choose it to lie half-way between the incident and final directions, i. e., we choose

$$\hat{\vec{R}} = \frac{\vec{k} + \vec{k}'}{|\vec{k} + \vec{k}'|} . \quad (89)$$

The revised approximation thus represents a wave scattered from a direction \vec{k}' to a direction \vec{k}' as undergoing, in travelling through a potential, phase shifts which are appropriate to a path deflected through half the final scattering angle, (see Fig. 2). This is evidently a crude correction for some of the bending of particle paths that takes place within the potential. The determination of \vec{R} by means of Eq. (89) actually simplifies the evaluation of the integral Eq. (80) for the scattering amplitude since, as long as energy is conserved, \vec{R} is then perpendicular to $\vec{k}-\vec{k}'$ i. e.,

$$(\vec{k}-\vec{k}') \cdot (\vec{k}+\vec{k}') = k^2 - k'^2 = 0 . \quad (90)$$

With this alteration, the scattering amplitude for an axially symmetric potential becomes

$$f(\theta) = \frac{k}{t} \int_0^\infty J_0(2kb \sin \frac{\theta}{2}) \{e^{iX(b)} - 1\} b db , \quad (91)$$

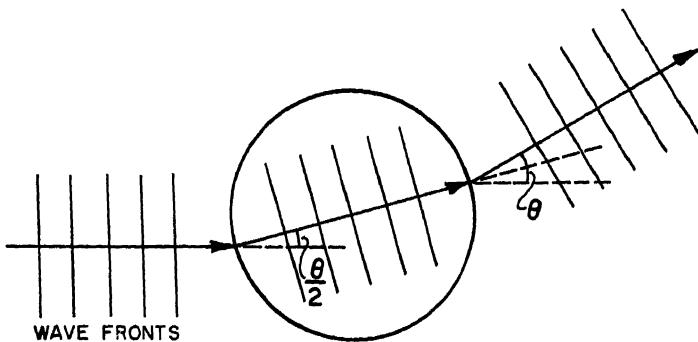


Fig. 2

i. e., the only change is to replace θ in the argument of the Bessel function by

$$2 \sin \frac{\theta}{2}.$$

To the extent that we restrict ourselves to the consideration of very small angles the change described is hardly a very great one. But it must be remembered that the angular distributions of scattering we are dealing with are peaked near the forward direction and as a consequence vary rapidly with angle. Even so slight a shift of the angular scale at small angles as we have just described may be of significance in improving the angular range over which the approximation holds, although, of course, the order-of-magnitude inequalities Eq. (87) and Eq. (88) still apply.

Further arguments in favor of the accuracy of Eq. (91) may be adduced. In particular, if the exponential, $\exp[i\chi(b)]$, is expanded in a power series, the successive terms correspond to the various orders of the Born approximation. In the form Eq. (91) the first Born amplitude is reproduced precisely for all θ so that the approximations characteristic of the high-energy procedure are confined to the second and higher order amplitudes. Still another indication of the accuracy of Eq. (91) will be encountered in showing its correspondence with the phase shift series.

An important test of the self-consistency of the high-energy approximation is furnished by the unitarity theorem (22). To illustrate this we shall present a rather simplified check of the optical, or conservation, theorem. According to this theorem, the total scattering

cross section should be given by

$$\sigma_{\text{tot.}} = \frac{4\pi}{k} \text{Im} f(k, k).$$

Now the expression for the scattering amplitude is

$$f(k', k) = \frac{k}{2\pi i} \int e^{i(k-k') \cdot b} \{ e^{iX(b)} - 1 \} d^{(2)}b,$$

so that the total cross section should be

$$\sigma_{\text{tot.}} = 2 \int (1 - \text{Re } e^{iX(b)}) d^{(2)}b. \quad (92)$$

To verify this expression we must integrate the differential cross section over the sphere $|k'| = k$

$$\begin{aligned} \int |f(k', k)|^2 d\Omega_{k'} &= \\ &= \left(\frac{k}{2\pi}\right)^2 \int e^{i(k-k') \cdot (b-b')} \{ e^{iX(b)} - 1 \} \{ \bar{e}^{iX(\bar{b})} - 1 \} d^{(2)}b d^{(2)}\bar{b} d\Omega_{k'}. \end{aligned} \quad (93)$$

Now to make a quick estimate of this integral we shall take advantage of the fact that the scattering is concentrated near the forward direction. We shall replace the integration over the sphere $|k'| = k$ by an integration over the plane in k' -space which is tangent to the sphere at $k' = k$, i. e., in the forward direction. In this case we may write

$$d\Omega_{k'} \approx \frac{d^{(2)}k'}{k'^2}, \quad (94)$$

where the differential element $d^{(2)}k'$ lies in a plane perpendicular to k' . Furthermore, we note that

$$\int e^{i(k-k') \cdot (b-b')} d^{(2)}k' = (2\pi)^2 \delta^{(2)}(b-b'), \quad (95)$$

where $\delta^{(2)}(b-b')$ is a two dimensional delta-function.

By carrying out the angular integration in this approximate way, we find

$$\sigma_{\text{scatt.}} = \int |e^{iX(b)} - 1|^2 d^{(2)}b. \quad (96)$$

Hence for \mathbf{X} real, i. e., in the absence of absorption, we have

$$\sigma_{\text{scatt.}} = 2 \int (1 - \text{Re } e^{iX(\mathbf{b})}) d^{(2)}\mathbf{b}, \quad (97)$$

which indeed agrees with the expression Eq. (92) obtained from the conservation theorem. It is a simple matter to extend the foregoing proof to include the cases $\mathbf{k}' \neq \mathbf{k}$ of the unitarity theorem Eq. (22), as long as \mathbf{k} and \mathbf{k}' lie close together in direction. Furthermore the proof may be improved considerably in accuracy by the introduction of a more precise means of carrying out the angular integration. That can be accomplished by taking the angular dependence of amplitude (91) quite literally and making use of the orthogonality relations for Bessel functions in evaluating the integral, Eq. (93).

As a by-product of the foregoing analysis we may derive an expression for the absorption cross section which is present if the phase shifts are complex. We have only to subtract expression Eq. (97) for the scattering cross section from Eq. (92) for the total cross section;

$$\begin{aligned} \sigma_{\text{abs.}} &= \sigma_{\text{tot}} - \sigma_{\text{scatt.}} \\ &= \int (1 - |e^{iX(\mathbf{b})}|^2) d^{(2)}\mathbf{b}. \end{aligned} \quad (98)$$

Relation of the High-Energy Approximation to Other Methods

It may improve our perspective a bit to show how the approximation we have been discussing is related to the various approaches mentioned earlier. The correspondence of the method with the Born approximation approach, has already been indicated. The power series expansion of

$$\exp[iX(\mathbf{b})]$$

on which the correspondence is based is only useful for

$$V_a/\hbar v \ll 1.$$

The W. K. B. limit,

$$V_a/\hbar v \gg 1,$$

is also implicitly contained in the approximation. In this limit the phase shift function is large in absolute magnitude compared with unity, so that the function

$$\exp[iX(\mathbf{b})]$$

oscillates rapidly. Now for any particular direction of scattering we must integrate the expression

$$\exp[i(\vec{k} - \vec{k}') \cdot \vec{b} + i\chi(b)]$$

over the \vec{b} -plane. Now in the classical limit this expression will oscillate so rapidly that the only appreciable contributions to the integral will come from the points of stationary phase. These, by symmetry, must lie in the plane containing \vec{k} and \vec{k}' . It is easy to verify that these stationary points represent just the classical impact vectors of particles scattered in the direction \vec{k}' . For the simpler choices of scattering potential there is usually only one stationary point for each \vec{k}' ; but there are, of course, potentials for which more than one classical path is possible and others for which there is none for scattering in certain directions. It is an elementary matter to integrate the expression for the scattering amplitude using the method of stationary phase. The result, at small angles, agrees with the W. K. B. approximation.

The correspondence of the high-energy approximation with the partial wave expansion becomes clear on comparing the expressions, Eq. (96) and Eq. (35), for the scattering cross sections. In the high-energy approximation the summation over angular momenta is replaced by an integration over impact vectors. If we adopt the asymptotic correspondence

$$kb \longleftrightarrow l + \frac{1}{2}, \quad (99)$$

the summation and integration become identical in form. The coefficients

$$C_l = e^{2i\delta_l}$$

must then be identified with the factors

$$e^{i\chi(b)},$$

so that we have the correspondence

$$\chi\left(\frac{l + \frac{1}{2}}{k}\right) \longleftrightarrow 2\delta_l. \quad (100)$$

These correspondences may be illustrated, for example, with the absorption cross section Eq. (37)

$$\frac{\pi}{k^2} \sum_l (2l+1)(1 - |e^{2i\delta_l}|^2) \longleftrightarrow \frac{\pi}{k^2} \int 2kbkdb (1 - |e^{i\chi(b)}|^2)$$

$$\longleftrightarrow \int (1 - |e^{iX(b)}|^2) d^{\omega}b.$$

To show the correspondence of the partial wave expansion for the scattering amplitude,

$$f(\theta) = \frac{1}{2ik} \sum_l (2l+1) \{ e^{2i\delta_l} - 1 \} P_l(\cos\theta), \quad (101)$$

with the high-energy approximation, we require an approximate form for the Legendre polynomials at small angles.

Now, in spherical coordinates, regions far from the origin and close to the polar axis are described in a way which differs only very slightly from that of cylindrical coordinates. Consequently, there is an approximate correspondence between the solution of the wave equation in the two systems. This correspondence may be expressed by the asymptotic relation

$$P_l(\cos\theta) \sim J_0(2(l+\frac{1}{2})\sin\frac{\theta}{2}) + \frac{1}{4} \sin^2\frac{\theta}{2} + \dots \quad (102)$$

Although this relation is most accurate for large l and small angles, the remainder term adds only a 6 per cent correction for $l=0$ and $\theta=60^\circ$. By discarding the remainder term and using the previously noted correspondences, we may reduce the partial wave expression Eq. (101) to precisely the form Eq. (92) of the high-energy expansion. The expansion Eq. (102) is seen to furnish some additional weight for the use of the argument

$$2 \sin\frac{\theta}{2}$$

rather than θ in the Bessel function.

Some Illustrative Examples

Before we proceed to generalize the high-energy approximation in various ways, it may be helpful to illustrate its use in some concrete examples. The simplest of these is one familiar from diffraction theory. We consider the case of an absorptive (i. e., negative imaginary) potential which is confined to a sphere of radius a , one which absorbs effectively enough that the sphere may be considered opaque. Note that the absolute value of the imaginary potential need not be very large to produce this effect. Even if the potential is only weakly absorptive in any volume element, it will be opaque if its radius is large enough.

Assuming the sphere to be opaque, we write

$$e^{iX(b)} = \begin{cases} 0 & , b < a \\ 1 & , b > a \end{cases}, \quad (103)$$

so that the scattering amplitude becomes

$$\begin{aligned} f(\theta) &= -\frac{k}{i} \int_0^a J_0(2kb \sin \frac{\theta}{2}) b db \\ &= i a \frac{J_1(2ka \sin \theta/2)}{2 \sin \theta/2}. \end{aligned} \quad (104)$$

The differential scattering cross section is thus

$$|f(\theta)|^2 = (ka^2)^2 \frac{J_1^2(2ka \sin \theta/2)}{[2ka \sin \theta/2]^2}, \quad (105)$$

which has the appearance typical of a short-wavelength diffraction pattern, shown in Fig. 3.

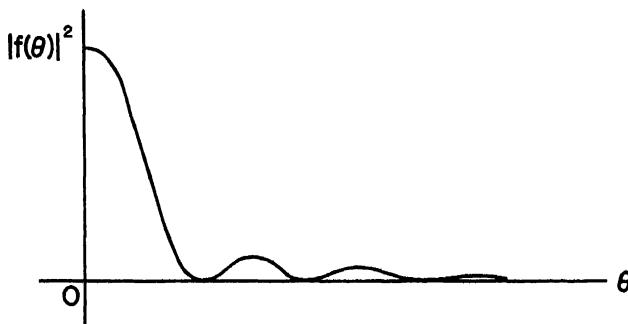


Fig. 3

The total scattering cross section is given simply by

$$\sigma_{\text{scatt.}} = \int |e^{iX(b)} - 1|^2 d^{(2)}b = \pi a^2, \quad (106)$$

since the only nonzero contribution to the integral comes from the shadow region, $b < a$. For the same reason we have

$$\sigma_{\text{abs.}} = \int (1 - |e^{iX}|^2) d^{(2)}b = \pi a^2 , \quad (107)$$

and

$$\sigma_{\text{tot.}} = 2 \int (1 - \text{Re } e^{iX}) d^{(2)}b = 2\pi a^2 . \quad (108)$$

The latter result is just twice the classical absorption cross section. The small-angle scattering, i. e., the intensity diffracted about the edges of the sphere, is of course, the non-classical effect responsible for the factor of two. Note that nothing essential in the discussion above rests on the choice of spherical shape of the potential. The scattering cross section will equal the absorption cross section for an opaque potential of any shape whose dimensions are large compared with the wavelength.

As a somewhat more general example let us consider the case of a square potential well of radius a ;

$$V(r) = \begin{cases} V_0 & , r < a \\ 0 & , r > a \end{cases} . \quad (109)$$

The phase shift function is then

$$\chi(b) = \begin{cases} -\frac{2V_0}{\hbar v} \sqrt{a^2 - b^2} & , b < a \\ 0 & , b > a \end{cases} . \quad (110)$$

In this case there is no longer any elementary way of carrying out the impact parameter integration to find the angular dependence of the scattering amplitude. The integral is best treated by means of a series expansion, due to I. Shapiro,⁸ which is a bit too lengthy to present here. The integration required to find the amplitude for scattering in the forward direction, however, may easily be carried out in closed form, and from the imaginary part of this amplitude we secure an expression for the total cross section.

In terms of the parameter

$$\alpha = \frac{V_0 a}{\hbar v} \quad (\text{V}_0 \text{ real}) \quad (111)$$

the ratio of the total scattering cross section to the geometrical cross section may be written as

$$\frac{\sigma_{\text{tot}}}{\pi a^2} = 2 + \frac{1}{\alpha^2} + \frac{2}{\alpha} \left(\frac{\cos 2\alpha}{2\alpha} + \sin 2\alpha \right). \quad (112)$$

A plot of

$$\sigma_{\text{tot}} / \pi a^2$$

versus α is shown in Fig. 4. It is of particular interest to note the limiting values

$$\frac{\sigma_{\text{tot}}}{\pi a^2} = \begin{cases} 2\alpha^2 & \text{for } \alpha \ll 1 \\ 2 & \text{as } \alpha \rightarrow \infty \end{cases}. \quad (113)$$

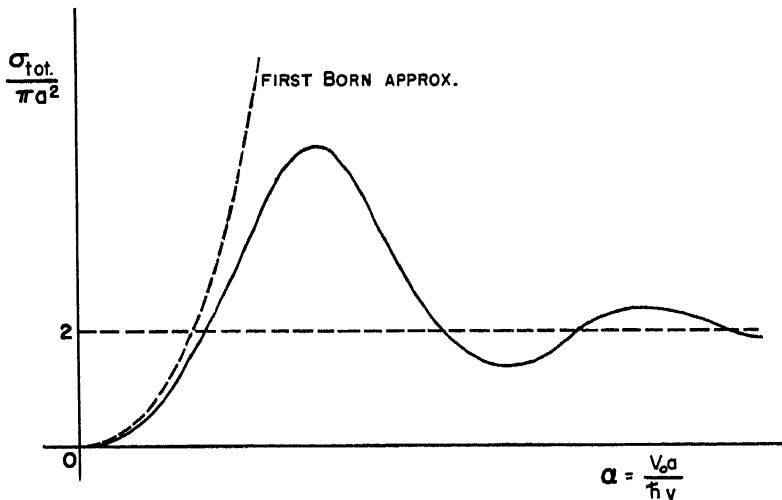


Fig. 4

The first of these is the Born approximation. The ratio 2 which appears in the limit

$$V_0 a / \hbar v \rightarrow \infty$$

is due to the contributions of two different types of scattering. Particles may be scattered either by penetrating the sphere and suffering relatively large deflections

$$\Theta \sim |V_0|/E$$

or by being diffracted about it and suffering relatively small ones,

$$\Theta \sim \frac{1}{ka}.$$

For the case of a Gaussian potential

$$V(r) = V_0 e^{-r^2/a^2} \quad (V_0 \text{ real}) \quad (114)$$

it is also easy to obtain the expression for the integrated scattering cross section. If again we write

$$\alpha = V_0 a / \hbar v$$

the result may be expressed as

$$\frac{\sigma_{\text{scatt.}}}{\pi a^2} = 2 \int_0^{\sqrt{\pi}\alpha} \frac{1 - \cos t}{t} dt \quad (115)$$

which is shown plotted as a function of α in Fig. 5. In this case, the

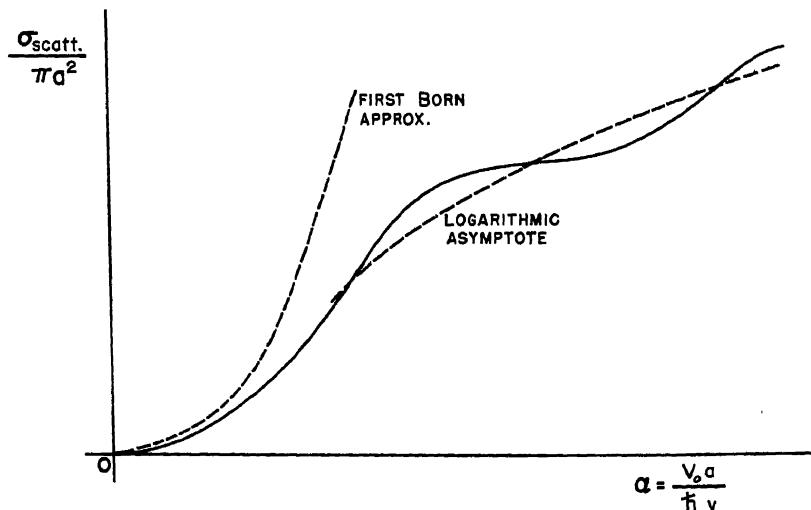


Fig. 5

values for small and large α are

$$\frac{\sigma_{\text{scatt.}}}{\pi a^2} = \begin{cases} \frac{\pi}{2} \alpha^2 & \text{for } \alpha \ll 1 \\ 2 \{ \log(\sqrt{\pi} \alpha) + .577 + \dots \} & \text{for } \alpha \gg 1 \end{cases} \quad (116)$$

The interesting point here is that in the limit

$$\alpha = V_0 a / \hbar v \rightarrow \infty$$

the ratio

$$\frac{\sigma_{\text{scatt.}}}{\pi a^2}$$

increases without bound. This may be a bit surprising since the decrease of the Gaussian potential with distance is notoriously rapid. The explanation lies in the fact that the limit

$$\frac{V_0 a}{\hbar v} \rightarrow \infty$$

is, in effect, the classical limit $\hbar \rightarrow 0$. The infinite value approached by the cross section is common to all potentials which possess gradients, however small, at unbounded distances from the origin. In the classical limit all particles passing through such potentials must be considered as scattered no matter how small the scattering angle may be. Hence, a potential with an infinitely extended tail will always lead to an infinite scattering cross section in the classical limit.

An example which is of considerable practical value is furnished by the Coulomb potential,

$$V(r) = Ze^2/r.$$

In this case, however, we are immediately confronted by the difficulty that the integral which represents the phase shift,

$$\chi(b) = - \frac{Ze^2}{\hbar v} \int_{-\infty}^{\infty} \frac{dz}{\sqrt{b^2 + z^2}} \quad ,$$

diverges logarithmically at both extremes of the range of integration. The difficulty here is essentially one common to all methods of approximation which assume that the incident wave is simply a plane wave. The slow decrease of the Coulomb field with distance has the effect that an

incoming wave is appreciably distorted in phase at large distances from the center of force. The only consistent way to treat scattering by a field which decreases so slowly would be to take this distortion into account.

Now in actual practice, scattering experiments virtually never involve Coulomb fields which decrease so very slowly. It is almost always possible to say that the charge in question is neutralized within a certain distance by surrounding charges of opposite sign. Usually this distance is quite small compared with laboratory dimensions, and it is often large compared with the particle wavelengths. This is typically the case, for example, in nuclear scattering experiments, where the distance in question is simply the atomic radius. Now in such cases, the difficulty noted above is no longer present. The field falls off rapidly enough with distance to permit an elementary application of the approximation method.

The screened Coulomb potential, we may assume, can be written in the form

$$\nabla(r) = \frac{Ze^2}{r} F(r) \quad (117)$$

where

$$F(r) \longrightarrow 0$$

as

$$r \longrightarrow \infty$$

a property which insures the convergence of the integral for $\chi(b)$. In order to secure a simple illustration we may consider the particular choice

$$F(r) = \begin{cases} 1, & r < a \\ 0, & r > a \end{cases}, \quad (118)$$

which leads to the phase shift function

$$\chi(b) = \begin{cases} -2 \frac{Ze^2}{\hbar v} \log\left(\frac{a + \sqrt{a^2 - b^2}}{b}\right), & b < a \\ 0, & b > a \end{cases} \quad (119)$$

The scattering amplitude which we wish to calculate is given by the expression

$$f(\theta) = \frac{k}{i} \int_0^\infty J_0(2kb \sin \theta/2) \{e^{i\chi(b)} - 1\} b db. \quad (91)$$

The integral required is not an elementary one, but it may be simplified appreciably by considering the limit of large screening radii,

$$ka \longrightarrow \infty.$$

This limit, in fact, represents well the situation which prevails in most nuclear scattering problems, where ka usually exceeds 10^5 . Now it is easy to see that in such cases the effect of the screening on the scattered intensity is virtually imperceptible. The screening affects particles whose impact parameters exceed the radius a , and so alters the scattered intensity only at the unobservably small angles,

$$\Theta \sim 1/ka.$$

Particles which are deflected to angles appreciably larger than this are ones which have suffered close encounters with the Coulomb field. We should therefore expect the Rutherford formula to hold for the intensity at angles

$$\Theta \gg 1/ka,$$

and we shall try to show that this is so.

To carry out the integration for the scattering amplitude, it helps to note that the integral

$$\int_0^\infty J_0(2kb \sin \theta/2) b db = \frac{1}{2\pi} \int e^{i(k-k') \cdot \vec{b}} d^2 b$$

is simply a two dimensional delta-function which vanishes for $k' \neq k$. Hence for angles $\theta \neq 0$ we need only calculate the integral

$$f(\theta) = \frac{k}{l} \int_0^\infty J_0(2kb \sin \theta/2) e^{iX(b)} b db, \quad (\theta \neq 0). \quad (120)$$

Now, because of the way in which the Bessel function oscillates, the most significant contributions to this integral will come from the region

$$b \sim 1/k\theta.$$

In this region we have

$$b/a \sim 1/ka\theta.$$

If we restrict the calculation to angles

$$\Theta \gg 1/ka,$$

we evidently have

$$b/a \ll 1$$

in the region which contributes most. We therefore evaluate the integral by expanding $\chi(b)$ in powers of b/a . The expansion of χ is

$$\chi(b) = 2 \frac{Ze^2}{\hbar v} \log \frac{b}{2a} + \frac{Ze^2}{\hbar v} \frac{b^2}{2a^2} + O\left(\frac{b^4}{a^4}\right). \quad (121)$$

The approximation of $\chi(b)$ by the first term of this series leads to an integral, Eq. (120), of a form which is well known. The scattering amplitude which results is

$$f(\theta) = - \frac{2k \frac{Ze^2}{\hbar v}}{(2k \sin \theta/2)^2} e^{-i\left\{2 \frac{Ze^2}{\hbar v} \log(2ka \sin \theta/2) - 2\eta\right\}} \quad (122)$$

where η is the phase angle

$$\eta = \arg \Gamma\left(1 + i \frac{Ze^2}{\hbar v}\right) \quad (123)$$

We have thus verified that for angles

$$\Theta \gg 1/ka$$

the scattered intensity

$$|f(\theta)|^2$$

indeed follows the Rutherford formula. The only effect of the screening on the scattering amplitude at these angles is the addition of a constant to its complex phase angle, which otherwise also agrees with the exact result for a Coulomb field. This phase constant contains the term

$$2 \frac{Ze^2}{\hbar v} \log ka$$

which must occur whatever the form of the screening function $F(r)$, and to it there is added in general a constant term, independent of the screen-

ing radius, but which does depend on the shape of the screening function.

For example, if we had chosen the screening function

$$F(r) = e^{-r/a} \quad (124)$$

the resulting scattering amplitude for

$$\Theta \gg 1/ka$$

would be precisely the result Eq. (122) multiplied by the phase factor

$$e^{2i \frac{Ze^2}{\hbar v} C}$$

where C is Euler's constant ($C= .577$).

In the foregoing discussion we have shown that the introduction of screening to a Coulomb field makes it possible for the high-energy approximation to solve the scattering problem accurately. If the screening radius a is large, the effect of screening on the intensities scattered to angles

$$\Theta \gg 1/ka$$

is negligible. The specific manner in which the field is screened affects only a multiplicative phase factor in the scattering amplitude. Now in applications to nuclear physics we are virtually never interested in the overall phase of the scattering amplitude when dealing with charged particles. This phase could, in principle, be measured through interference effects, but our discussion shows that it is more sensitive to atomic parameters than to nuclear ones, and hence is not of great interest. Since few nuclear measurements are sensitive to the effects of screening, it ordinarily makes little difference what form the screening is assumed to take.

In nuclear applications, the incident particle is usually subject to nuclear forces as well as to the Coulomb field. The use of the method for such cases requires only that the phase shift functions $\chi(b)$ for the nuclear and Coulomb interactions be superposed, i. e., the nuclear phase shift function is added to Eq. (121) and the sum substituted for $\chi(b)$ in Eq. (120). The amplitude calculated in this way takes proper account of the two kinds of scattering plus all of the interferences that occur between them.

Treatment of More General Static Interactions

Before passing on to the treatment of time-varying potentials and the many-body problem, it will be helpful to indicate how the high-energy approximation may be applied to spin-dependent and velocity-dependent

interactions. We shall suppose that the incident particle has spin 1/2, and shall represent its angular momentum vector (in units of \hbar) by

$$\vec{S} = \frac{1}{2} \vec{\sigma}$$

where $\vec{\sigma}$ is the familiar Pauli spin vector

$$\sigma_i \sigma_j + \sigma_j \sigma_i = 2\delta_{ij}.$$

The orbital angular momentum of the particle (in units of \hbar) is represented by the operator

$$\vec{L} = \frac{1}{\hbar} (\vec{r} \times \vec{p}).$$

A particular form of nuclear interaction which possesses all of the required invariances and is both spin and velocity dependent may be obtained by multiplying the scalar product $\vec{\sigma} \cdot \vec{L}$ by any spherically symmetric function of position. More generally we may consider an interaction made up of a central potential $V_c(r)$ and a spin-orbit potential $(\vec{\sigma} \cdot \vec{L})V_s(r)$,

$$V(r) = V_c(r) + V_s(r) \vec{\sigma} \cdot \vec{L}. \quad (125)$$

The treatment of this potential¹¹ will be of use to us both to illustrate the method and to serve, at a later point, as a means of identifying the spin-orbit potential which is effective in the many-body problem.

In order to generalize the approximation to include the spin variable, we shall write the wave function in the form

$$\Psi_k(\vec{r}) = e^{i\vec{k} \cdot \vec{r}} \varphi(\vec{r}) u_i, \quad (126)$$

where u_i is a two-component spinor representing the initial state of the particle, and $\varphi(\vec{r})$ is an operator which induces the appropriate change of spin state. By making the approximations described earlier, and further assuming

$$|V_s|/E \ll 1,$$

the equation determining $\varphi(\vec{r})$ may be reduced once again to the form Eq. (72). Its solution is

$$\varphi(\vec{r}) = e^{-\frac{i}{\hbar v} \int_{-\infty}^z \{ V_c(\vec{b} + \hat{k} z') + V_s(\vec{b} + \hat{k} z) \vec{\sigma} \cdot (\vec{b} \times \hat{k}) k \} dz'} \quad (127)$$

Again by a procedure of the type described earlier we may use the expression for $\varphi(\vec{r})$ to derive the scattering amplitude,

$$f(k', k) = \frac{k}{2\pi i} \int e^{i(\vec{k}-\vec{k}') \cdot \vec{b}} \{ e^{iX_c(\vec{b}) + iX_s(\vec{b}) \vec{\sigma} \cdot (\vec{b} \times \hat{k}) k} - 1 \} d^{(2)}b. \quad (128)$$

Here X_c and X_s are the phase shifts

$$X_c(\vec{b}) = -\frac{1}{\hbar v} \int_{-\infty}^{\infty} V_c(\vec{b} + \hat{k} z') dz', \quad X_s(\vec{b}) = -\frac{1}{\hbar v} \int_{-\infty}^{\infty} V_s(\vec{b} + \hat{k} z') dz'. \quad (129)$$

Now the exponential containing the spin operator in the integrand of Eq. (128) is considerably simpler in structure than it may appear. In fact, any function whatever of $\vec{\sigma}$ must reduce to a linear function. In the above case the reduction is easily verified by using the anticommutation rule to simplify the power series expansion. The scattering amplitude may then be written in the form

$$f(k', k) = \frac{ik}{2\pi} \int e^{i(\vec{k}-\vec{k}') \cdot \vec{b}} \{ \Gamma_c(\vec{b}) + i\vec{\sigma} \cdot \left(\frac{\vec{b}}{b} \times \hat{k} \right) \Gamma_s(\vec{b}) \} d^{(2)}b, \quad (130)$$

where Γ_c and Γ_s are the axially symmetric functions

$$\Gamma_c(\vec{b}) = 1 - e^{iX_c(\vec{b})} \cos[kbX_s(\vec{b})] \quad (131)$$

$$\Gamma_s(\vec{b}) = -e^{iX_c(\vec{b})} \sin[kbX_s(\vec{b})]. \quad (132)$$

The scattering amplitude we are constructing is to be regarded as an operator which transforms the initial spin state of the particle into its final state. As such, the most general form it can take is

$$f(k', k) = f(k', k) + (\vec{\sigma} \cdot \vec{n}) g(k', k), \quad (133)$$

where f and g are spin-independent amplitudes and \vec{n} is a unit vector perpendicular to the plane of scattering.

$$\hat{n} = \frac{\vec{k} \times \vec{k}'}{|\vec{k} \times \vec{k}'|} . \quad (134)$$

By carrying out the integration of Eq. (130) over the azimuthal angle we find

$$f(k', k) = ik \int_0^\infty J_1(|\vec{k} - \vec{k}'| b) \Gamma_c(\xi) b db \quad (135)$$

+

$$g(k', k) = -ik \int_0^\infty J_1(|\vec{k} - \vec{k}'| b) \Gamma_s(\xi) b db . \quad (136)$$

The appearance of the Bessel function J_1 in the latter integral is due to dependence of the spin-orbit potential on the azimuthal angle. The amplitude g may be seen to vanish for forward scattering, as it must, since in that case there is no longer any axial vector to represent a possible direction of spin polarization. The particles scattered at nonvanishing angles are in general polarized. The effect which gives rise to the polarization may be thought of as a species of double refraction caused by the spin dependence of the interaction.

It is also of interest to consider more general forms of operator-dependent interactions. We shall suppose, for simplicity, that the problem is one-dimensional, and that we are given an interaction operator $V(x)$. The equation for the modulating function $\varphi(x)$ is, as before,

$$\frac{d\varphi(x)}{dx} = -\frac{i}{\hbar v} V(x) \varphi(x) , \quad (53)$$

but where questions of commutation are concerned we must exercise care in integrating it. In particular if the values of the operator-function $V(x)$ do not commute with one another for all x , it is no longer correct to write the solution to Eq. (53) as a simple exponential. It is possible, however, to write the solution to Eq. (53) as a power series

$$\varphi(x) = 1 - \frac{i}{\hbar v} \int_{-\infty}^x V(x') dx' + \left(\frac{i}{\hbar v} \right)^2 \int_{-\infty}^x dx' \int_{-\infty}^{x'} V(x') V(x'') dx'' + \dots . \quad (137)$$

When the operators commute, the expansion is simply that of the exponential

$$\exp \left[-\frac{i}{\hbar v} \int_{-\infty}^x V(x') dx' \right] .$$

When the operators fail to commute, we shall introduce for the series (137) the notation

$$\varphi(x) = \left\{ e^{-\frac{i}{\hbar v} \int_{-\infty}^x V(x') dx'} \right\}_+ . \quad (138)$$

The bracket $\{ \}_+$ is to be taken to mean that in the successive terms of the power series expansion the operators $V(x)$ are written in order of increasing argument from right to left.

A corresponding notation may be introduced in the three-dimensional problem. The formal expression for the scattering amplitude which one finds requires that the expression $\exp[iX(b)]$ in the integrand be replaced by the more general form

$$\left\{ e^{-\frac{i}{\hbar v} \int_{-\infty}^{\infty} V(b + \hat{k}z) dz} \right\}_+ . \quad (139)$$

This expression reduces to the simple exponential whenever the different values of the potential along a straight-line path commute with one another (as they do for example to first order in V/E for a spin-orbit potential). An example for which the more general formulation is required is furnished by the tensor force between two nucleons.

Time-dependent Interactions

When the systems with which the incident particle interacts are no longer inert their influence on the particle becomes time-dependent. The simplest case to treat is the interaction of the particle with a time-dependent external field, $V(x, t)$. Once again we consider a problem with only one spatial dimension so that the time-dependent Schrödinger equation is

$$\left(\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + i\hbar \frac{\partial}{\partial t} \right) \psi(x, t) = V(x, t) \psi(x, t) , \quad (140)$$

and the wave function may be written in the form

$$\psi(x, t) = e^{i(kx - \omega t)} \varphi(x, t) , \quad (141)$$

where $\omega = E/\hbar = \hbar k^2/2m$. The approximation we make is once again the assumption that $\varphi(x, t)$ varies slowly as a function of x . For this reason we again drop the term $i\hbar \partial \varphi / \partial x$ from the Schrödinger equation, and find the equation for φ ,

$$\left(\frac{\partial}{\partial x} + \frac{1}{v} \frac{\partial}{\partial t} \right) \varphi(x, t) = -\frac{i}{\hbar v} V(x, t) \varphi(x, t) . \quad (142)$$

This equation is easily reduced to a form similar to Eq. (53) by introducing as an independent variable the quantity $s=t-x/v$, and using it to replace t . We shall assume that a steady plane wave is incident, which originates at $x = -\infty$. Since the approximation neglects reflection, the boundary condition on φ is $\varphi(-\infty, t) = 1$ for all t . The solution to Eq. (142) which applies in this case is

$$\varphi(x, t) = e^{-\frac{i}{\hbar v} \int_{-\infty}^x V(x', t - \frac{x-x'}{v}) dx'}, \quad (143)$$

i.e., in integrating the potential to find the shift of phase of the wave function, the potential must be evaluated for each point at the time corresponding to the passage of the particle.

Since the function φ is explicitly time-dependent the wave function $\psi(x, t)$ will no longer depend on time simply as $\exp[-i\omega t]$. The introduction of other Fourier components into the time dependence means that particles are scattered inelastically. It also implies certain restrictions on the validity of the approximation (143) which must be added to those discussed earlier.

The approximation is consistently one which assumes that the momentum change of the incident particle is small. When inelastic scattering is present it must be assumed that the change in the absolute value of the momentum is small (as well as any change in direction that may take place in three dimensions). Hence the approximation is only valid for scattering which is not too strongly inelastic, $\Delta E/E \ll 1$. For this reason we must restrict consideration to fields $V(x, t)$ whose dominant frequencies are much smaller than ω .

It is also of interest to generalize the approximation to the case in which the values of the interaction operator fail to commute at the different points along a trajectory. This would be the case, for example, for a particle traversing a region containing a quantized field. The solution for $\varphi(x, t)$ in such a case is

$$\varphi(x, t) = \left\{ e^{-\frac{i}{\hbar v} \int_{-\infty}^x V(x', t - \frac{x-x'}{v}) dx'} \right\}_+, \quad (144)$$

where the ordering bracket refers, as before, to the variable x' . This expression is of use more generally; e.g. in considering collisions in which the target possesses internal degrees of freedom.

Scattering by a Bound Particle

The target particles in actual scattering experiments are always free to move about, to a certain degree, and to absorb recoil momentum. In nuclear and atomic experiments they are usually in a bound state of some sort initially, i.e., confined to the interior of a nucleus or molecule,

and may make transitions under the impact of the incident particle to states which are either free or bound. The approximation procedure we have been describing can be extended in a natural way to treat such problems. To illustrate this generalization we shall consider a one-dimensional problem which may be described as follows:

The target particle has coordinate q . Its Hamiltonian, $H(q)$, has eigenvalues ϵ_j which correspond to eigenstates U_j . It will be convenient to assume that at least one of these states, which we take to be the initial state U_i , is bound, and confines the particle to the neighborhood of the origin. The incident particle is described by the coordinate x , and is assumed to interact with the target particle via the potential $V(x-q)$. We shall assume that this potential satisfies the conditions for the high-energy approximation noted earlier.

In treating this problem, there is a certain formal convenience in being able to discuss separately the behavior of the incident and target particles. A procedure which allows this, in a measure, may be based on the time-dependent form of the Schroedinger equation. If we let Ω represent the time-dependent state of the system, this equation is

$$\left\{ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x-q) + H(q) \right\} \Omega = i\hbar \frac{\partial}{\partial t} \Omega . \quad (145)$$

Now let us assume that the dynamics of the unperturbed target particle are sufficiently well understood that its motion may be described in terms of time-dependent operators, i.e., via the Heisenberg picture. To secure such a description we remove from the state vector Ω the time dependence induced by the Hamiltonian $H(q)$, i.e., we introduce the state Ψ by means of the relation

$$\Omega = e^{-H(q)t/\hbar} \Psi . \quad (146)$$

Substituting this into the Schroedinger equation, we secure

$$\left\{ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + e^{iH(q)t/\hbar} V(x-q) e^{-iH(q)t/\hbar} \right\} \Psi = i\hbar \frac{\partial}{\partial t} \Psi . \quad (147)$$

We now define the time-dependent coordinate operator,

$$q(t) = e^{iH(q)t/\hbar} q e^{-iH(q)t/\hbar} . \quad (148)$$

Since the variables x and q commute, the Schroedinger equation reduces

to

$$\left\{ \frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + i\hbar \frac{\partial}{\partial t} \right\} \Psi = V(x - q(t)) \Psi . \quad (149)$$

This form of the equation is very similar in structure to Eq. (140) which we encountered in treating a particle moving through a time-dependent external field. The only difference arises from the fact that $q(t)$ is an operator whose values at different times do not in general commute. But we have already dealt with this complication at the end of the last section, and so the approximation procedure is now straightforward.

We write the wave function, by analogy with previous work, in the form

$$\Psi(x, t) = e^{i(kx - \omega t)} \varphi(x, t) u_i , \quad (150)$$

where u_i represents the initial state of the target, and φ is an operator implicitly dependent on q , which induces appropriate changes of the target state. With the approximations noted earlier, the equation determining φ is

$$\left(\frac{\partial}{\partial x} + \frac{i}{\hbar v} \frac{\partial}{\partial t} \right) \varphi(x, t) = - \frac{i}{\hbar v} V(x - q(t)) \varphi(x, t) . \quad (151)$$

The solution to this equation may be written as

$$\varphi(x, t) = \left\{ e^{-\frac{i}{\hbar v} \int_{-\infty}^x V(x' - q(t - \frac{x-x'}{v})) dx'} \right\}_+ . \quad (152)$$

This expression permits us to calculate, for example, the amplitude for the incident particle to be at the point x at time t when the target particle is at the same time in the state u_f . The amplitude is given by the scalar product

$$(u_f, \Psi(x, t)) = e^{i(kx - \omega t)} (u_f, \left\{ e^{-\frac{i}{\hbar v} \int_{-\infty}^x V(x' - q(t - \frac{x-x'}{v})) dx'} \right\}_+ u_i) . \quad (153)$$

Now, since we know the energies of the target states i and f , it is possible to simplify the x - and t -dependence of this expression. We make use of the definition (148) of the time-dependent coordinate operator to write

$$q(t - \frac{x-x'}{v}) = e^{i \frac{H(q)}{\hbar} (t - \frac{x}{v})} q_r(\frac{x'}{v}) e^{-i \frac{H(q)}{\hbar} (t - \frac{x}{v})}, \quad (154)$$

so that Eq. (153) may be reduced to the form

$$e^{i(kx - \omega t)} (u_f, e^{i \frac{H(q)}{\hbar} (t - \frac{x}{v})} \left[-i \frac{1}{\hbar v} \int_{-\infty}^x V(x' - q(\frac{x'}{v})) dx' \right]_+ e^{-i \frac{H(q)}{\hbar} (t - \frac{x}{v})}) \quad (155)$$

$$= e^{i[(k + \frac{\epsilon_i - \epsilon_f}{\hbar v})x - (\omega + \frac{\epsilon_i - \epsilon_f}{\hbar})t]} (u_f, \left[e^{-i \frac{1}{\hbar v} \int_x^\infty V(x' - q(\frac{x'}{v})) dx'} \right]_+ u_i).$$

This expression shows explicitly that the time dependence of the target coordinate is such as to preserve the conservation of energy and momentum, i.e., (155) is a wave function for the incident particle which accounts for the proper exchange of energy and momentum. Note however that the representation of the momentum change is only correct for small changes of energy, $|\epsilon_i - \epsilon_f|/E \ll 1$. This is precisely the limitation discussed in the preceding section.

In practice it would generally be extremely difficult to attempt an exact valuation of a time-ordered operator such as occurs in Eq. (155). In fact we rarely know enough about the operator $q(t)$, which describes the motion of the target particle to construct it explicitly. Since the expression (155) is already based upon certain approximations, there is no need to evaluate it to a high order of accuracy. Instead we may evaluate it by introducing a further approximation which is consistent with those made earlier and of comparable accuracy.

The point of departure of the approximation is the neglect of the time dependence of the operator $q(t)$. A sufficient condition for this neglect to be accurate may be seen from the Schrödinger equation (145). It is that the Hamiltonian $H(q)$ take on values which are small compared to the incident kinetic energy E . This must be true both for the initial bound state of the target and its final state whether bound or freely recoiling. In most applications the high-energy approximation is valid only for energies which are considerably larger than those characteristic of bound states of nuclei or atoms, so that the latter energies may be justifiably neglected. The Hamiltonian $H(q)$ must be restricted not only in its initial and final values, but must remain much smaller than E during the collision as well. For this reason the approximation only treats correctly collisions in which the momentum transfer is small. The condition that the momentum transferred be a small fraction of the incident momentum, i.e., that the

angle of scattering be small, is one of the assumptions already underlying the high-energy approximation. The calculations of the earlier sections assure us that at sufficiently high energies nearly all of the scattering will take place through small angles. The recoil momenta of the target particles will therefore be small and their energies quite small compared to E .

The effects of neglecting the time dependence of $q(t)$ may be seen in somewhat more detail in the expression (155). The exponential time dependence of Eq. (155) indicates the energy of the incident particle. One effect of neglecting the time dependence of $q(t)$ is the neglect of the energy increment, $\epsilon_i - \epsilon_f$, of the incident particle. This assumption, which is exact for elastic scattering, remains an accurate approximation for final states u_f which correspond to fairly inelastic collisions. The second consequence of dropping the time dependence of $q(t)$ lies in the neglect of what we may describe as a retardation effect, i.e., in Eq. (152) the operator q is evaluated at a time at which the incident particle is at x' , assuming that it reaches x at time t . The argument of q which occurs in Eq. (152) is simplified to the form x/v by the unitary transformation (154). The physical significance of this argument may be seen by considering the function $V(x' - q(\frac{x'}{v}))$ in its dependence upon the integration variable x' . If, for example, the target particle is moving in the same direction as the incident particle the effect of the x' -dependence of $q(x/v)$ is to increase the interval of the variable x' over which the interaction V extends. This dependence corrects for the fact that the velocity of the incident particle with respect to the target particle is different from its velocity in the laboratory system. Neglect of the retardation effect therefore requires that the velocity of the target particle be small compared to the velocity of the incident particle.

The neglect of retardation, of course, greatly simplifies the expression (155). Approximation of $q(x/v)$ by $q(0) = q$ means that the time ordering brackets may be removed and the expression between them regarded as a simple exponential. By neglecting the energy differences $\epsilon_i - \epsilon_f$ as a part of the same approximation we find

$$(u_f, \Psi(x,t)) = e^{i(kx-wt)} (u_f, e^{-\frac{i}{\hbar v} \int_{-\infty}^x V(x'-q) dx'}) u_i \quad (156)$$

This result could, of course, have been derived in fewer steps by neglecting $H(q)$ at an earlier stage of the argument. It is of some interest, however, to see the separation, as in Eq. (155), of the two conditions that the approximation hold, namely that the energy ratio $|\epsilon_i - \epsilon_f|/E$ and the ratio of the target and incident particle velocities both be much smaller than unity. The general expression (155) may be used to construct an expansion in powers of these parameters whose initial term is (156). We shall not derive these corrections here.

The foregoing calculations may be generalized directly to treat

three dimensional scattering problems. The approximation analogous to Eq. (156) for the time independent wave function in three dimensions is clearly

$$\Psi_{k,i}(\vec{r},\vec{q}) = e^{ik \cdot \vec{r} - \frac{i}{\hbar v} \int_{-\infty}^z V(\vec{b} + \hat{K} z' - \vec{q}) dz'} u_i(\vec{q}) . \quad (157)$$

To describe a collision we must specify the initial and final states, i and f , of the target particle as well as the initial and final propagation vectors, \vec{k} and \vec{k}' , of the incident particle. The corresponding scattering amplitude will be written as $F_{fi}(\vec{k}', \vec{k})$. An exact expression for this amplitude may be constructed in terms of the values of the two-particle wave function within the range of the potential $V(\vec{r} - \vec{q})$. The derivation is very similar to that of the expression Eq. (11) for the single particle amplitude, and the result forms an obvious generalization of it,

$$F_{fi}(\vec{k}', \vec{k}) = - \frac{2m}{4\pi\hbar^2} \int e^{-ik' \cdot \vec{r}} u_f^*(\vec{q}) V(\vec{r} - \vec{q}) \Psi_{k,i}(\vec{r}, \vec{q}) d\vec{r} d\vec{q} . \quad (158)$$

When the approximate wave function Eq. (157) is substituted in this expression, the integration over the coordinate z may be carried out precisely as in Eqs. (79) and (80). The result of this integration may be written in the form

$$F_{fi}(\vec{k}', \vec{k}) = \frac{k}{2\pi i} \int e^{i(\vec{k} - \vec{k}') \cdot \vec{b}} \int u_f^*(\vec{q}) [e^{i\chi(\vec{b} - \vec{s})} - 1] u_i(\vec{q}) d\vec{q} d^{(2)}b . \quad (159)$$

Here the coordinate \vec{s} represents the component of \vec{q} perpendicular to the propagation direction \hat{K} ,

$$\vec{s} = \vec{q} - \hat{K}(\hat{K} \cdot \vec{q}) , \quad (160)$$

and the phase shift function χ is given by

$$\chi(\vec{b} - \vec{s}) = -\frac{1}{\hbar v} \int_{-\infty}^{\infty} V(\vec{b} - \vec{s} + \hat{R}_z) dz . \quad (161)$$

This is simply the phase shift function discussed earlier, but with the impact parameter relative to a fixed center replaced by the impact parameter relative to the transverse coordinate \vec{s} of the target particle. Because of the infinite range of the z integration in Eq. (161) the phase shift is independent of the longitudinal coordinate $(\vec{K} \cdot \vec{q})$ of the target.

The expression (159) for the scattering amplitude will furnish the basic approximation for the considerations to follow. It may be shown by means of the expansion procedure discussed earlier that the corrections to cross sections calculated by means of Eq. (159) are of the same order as or smaller than those implicit in the high-energy approximation. In particular, for azimuthally symmetric bound states, the first corrections are of order θ^2 , (where the scattering angle θ is small) and of order v_t^2/v^2 where v_t is the velocity of the target particle in a bound state. If the bound states are not azimuthally symmetric, as may be the case, e. g., for oriented target nuclei, angular asymmetries of order θ may appear, but these are likewise weak corrections for the small-angle collisions under consideration.

Optical Theorem for Scattering by Bound Particles

We have maintained that when the incident particle energy is sufficiently high the simple approximation (159) represents accurately the amplitude for the overwhelming proportion of collision processes that actually occur, whether elastic or inelastic. A check on the self-consistency of this statement may be made by showing that Eq. (159) obeys the unitarity theorem. Here we shall limit ourselves to verifying the particular case of the optical theorem, since it is of use in establishing total cross sections.

The total cross section for collisions in which the target particle, originally in the state i , makes a transition to the state f is

$$\sigma_{fi} = \int \frac{k'}{k} |F_{fi}(\vec{k}', \vec{k})|^2 d\Omega_{k'} . \quad (162)$$

The factor k'/k in the integrand of this expression reduces to unity since we are neglecting the energy change of the incident particle.

The fact that the scattering is always concentrated near the forward direction enables us to carry out the integration of Eq. (162) much as we did for the case of scattering by a fixed potential. We replace the integration over the sphere $|\vec{k}'| = k$ by an integration over a plane tangent to the sphere at the point \vec{k} , which represents forward scattering, i. e.,

$$d\Omega_{k'} \longrightarrow \frac{d^{(2)}k}{k^2} .$$

In this way we find

$$\sigma_{fi} = \left(\frac{k}{2\pi}\right)^2 \iint e^{i(\vec{k}-\vec{k}') \cdot (\vec{b}-\vec{b}')} d^{(a)} b d^{(a)} b' \iint u_i^*(q') u_f(q') [e^{-iX(\vec{b}-\vec{s})} - 1].$$

$$[e^{iX(\vec{b}-\vec{s})} - 1] u_f^*(q) u_i(q) dq' dq \frac{d^{(a)} k'}{k^2} \quad (163)$$

$$= \int d^{(a)} b \iint u_i^*(q') u_f(q') [e^{-iX(\vec{b}-\vec{s})} - 1] [e^{iX(\vec{b}-\vec{s})} - 1] u_f^*(q) u_i(q) dq' dq,$$

where the representation Eq. (95) of the delta-function has been used in reaching the latter expression.

To find the total cross section for all types of collisions in which the target particle begins in the state i , we must sum (163) over all states f . The summation is easily carried out by using the completeness relation

$$\sum_f u_f(\vec{q}') u_f^*(\vec{q}) = \delta(\vec{q}' - \vec{q}), \quad (164)$$

so that we find

$$\begin{aligned} \sigma_{tot.} &= \sum_f \sigma_{fi} \\ &= \int d^{(a)} b \iint |u_i(\vec{q})|^2 |e^{iX(\vec{b}-\vec{s})} - 1|^2 d\vec{q} . \end{aligned} \quad (165)$$

Now, as long as there are no interactions which allow inelastic processes other than those we have described, the phase shift function $X(\vec{b} - \vec{s})$ will be real (or, more generally, a hermitian operator), so that Eq. (165) may be written as

$$\sigma_{tot.} = 2 \int d^{(a)} b \iint |u_i(\vec{q})|^2 [1 - \operatorname{Re} e^{iX(\vec{b}-\vec{s})}] d\vec{q} . \quad (166)$$

The latter expression when multiplied by $k/4\pi$ is seen to be just the elastic scattering amplitude in the forward direction, as given by Eq. (159). We have therefore verified the optical theorem

$$\sigma_{tot.} = \frac{4\pi}{k} \operatorname{Im} F_{ii}(\vec{k}, \vec{k}) . \quad (167)$$

An expression for the purely inelastic part of the total cross section may be obtained by subtracting the elastic cross section σ_{el} , as given by Eq. (163), from the expression (165) for σ_{tot} . In this way we obtain

$$\begin{aligned}\sigma_{inelast.} &= \sum_{f \neq i} \sigma_{fi} \\ &= \int d^{(2)} b \left\{ \int |u_i(q)|^2 |e^{iX(b-s)-1}|^2 dq - \left| \int |u_i(q)|^2 [e^{iX(b-s)-1}] dq \right|^2 \right\} \quad (168) \\ &= \int d^{(2)} b \left\{ \int |u_i(q)|^2 |e^{iX(b-s)}|^2 dq - \left| \int |u_i(q)|^2 e^{iX(b-s)} dq \right|^2 \right\}.\end{aligned}$$

If the phase shift function is real this expression reduces to

$$\sigma_{inelast.} = \int d^{(2)} b \left\{ 1 - \left| \int |u_i(q)|^2 e^{iX(b-s)} dq \right|^2 \right\}. \quad (169)$$

It is a bit premature to discuss the conditions under which the phase shift function may take on complex values, but it is worth mentioning that this may be the case when the interactions we have considered are not sufficient to describe the physical situation in all detail. If other interactions are present which lead to transitions of a type not accounted for above (e. g., meson production or particle-antiparticle annihilation), the phase shifts for simple scattering processes will in general be complex. Transitions in which particle numbers are not conserved have been omitted from the analysis, but the effect of their existence on the transitions which do conserve particle numbers will be felt through the alteration of the phase shift functions.

Scattering by a Many-Particle System

The conditions for the validity of the approximation we have been discussing do not, in fact, restrict the number of particles making up the target system. To use the same method to treat collisions with many-body systems we have only to require that the interactions between the target particles and the incident particle be of a form which may be treated by the high-energy approximation, and place the restrictions mentioned earlier on the bound state energies. The treatment of a many-body target then becomes a simple extension of that of a single bound particle. We have only to replace the single particle wave function by the many-particle wave function

$$\mathcal{U}(\vec{q}) \rightarrow \mathcal{U}(\vec{q}_1, \vec{q}_2, \dots, \vec{q}_N) \quad (170)$$

and the single-particle phase shift function (161) by the phase shift suffered by the incident particle in passing through a configuration of target particles. If the incident particle interacts with the target particles by means of two-body forces this phase shift is simply the sum of the phase shifts caused by the individual particles

$$X(\vec{b} - \vec{s}) \rightarrow \sum_{j=1}^N X_j(\vec{b} - \vec{s}_j) \quad (171)$$

The index j has been placed on the functions X since the interactions need not all be the same.

By using these more general expressions, we may write the amplitude for a scattering process in which the target system makes a transition from the state i to the state f as

$$F_{fi}(\vec{k}', \vec{k}) = \frac{k}{2\pi i} \int e^{i(\vec{k}' - \vec{k}) \cdot \vec{b}} d^3 b \cdot \\ \int \mathcal{U}_f(\vec{q}_1, \dots, \vec{q}_N) \left[e^{i \sum_{j=1}^N X_j(\vec{b} - \vec{s}_j)} - 1 \right] \mathcal{U}_i(\vec{q}_1, \dots, \vec{q}_N) T_j d\vec{q}_j \quad (172)$$

There is only one limitation on the validity of this expression which is of a type not already encountered in dealing with single-particle targets. We must require that the particles of the target system not be too far apart to prevent the use of the approximate wave functions on which the method is based. As we remarked in connection with Eq. (74), the approximate wave functions used are not intended to be accurate at large distances from the force centers. One may see, in fact, that their accuracy breaks down at distances of order $a^2/\lambda = ka^2$, where a is the force range. (A simple example which illustrates this is the breakdown of the geometrical shadow cast by a black sphere.) For this reason one must require that the target particles be contained within a radius R of one another obeying the inequality

$$R \ll ka^2. \quad (173)$$

Since the entire procedure is only applicable for $k\alpha \gg 1$, this condition is ordinarily satisfied for scattering by nuclei.

From the standpoint of the logic involved, no great innovation has been required to treat many-particle as well as single-particle targets. There is, however, a variety of ways of looking at the many-particle problem, and according to one of the more popular ones, what we have done can seem quite remarkable indeed. The method we refer to is one which views the incident particle as undergoing a succession of individual collisions with the different particles of the target system. The difficulties this method encounters stem from the close proximity of the target particles, and the obvious mathematical complication of treating multiple scattering. The closeness of the target particles means that the scattering amplitudes required for such calculations are not the ones measured experimentally. Furthermore, because of the evident difficulty of treating even double scattering, nearly all such work has been confined to the discussion of single-scattering, i.e., the scattering amplitude has been written as the sum of the amplitudes due to each of the target particles considered individually.

Now the expression (172) is no such simple superposition. We have added together the phase shifts produced by the individual target particles, not the scattering amplitudes. This means that multiple scattering effects are taken into account by Eq. (172). We shall presently demonstrate that it treats correctly even scatterings by all N particles in succession. Of course this is only to say that, under the conditions stated, the multiple scattering problem is less formidable than one usually imagines. The high-energy approximation, as we have noted, is, in fact, favored by the close proximity of the nucleons.

Eclipse-Effect in Deuterium

One of the simplest illustrations we can make of the theory outlined is the discussion of collisions between a single particle and a deuteron.¹² When the energy of the incident particle is so high that its wavelength is much smaller than the deuteron radius one might presume, rather naively as it develops, that the neutron and proton scatter independently and that the deuteron cross section is simply the sum of their two cross sections. Experiments have shown, however, that even at extremely high energies the various cross sections of the deuteron deviate measurably from the assumed additive rule. Such deviations have been found in experiments involving beams of incident nucleons, mesons, and anti-protons, and appear to be dramatically large in the latter case. A very crude model may serve to illustrate the way in which this comes about.

At energies of the order of 1 bev or higher colliding nucleons engage in meson production about as often as they scatter elastically. That means that if we confine our attention to collisions which conserve particle numbers, we may not be too far wrong in thinking of nucleons as being quite absorptive. We might think of their region of interaction, say, as a black sphere having a total cross section which is twice its absorp-

tion cross section.

Now the absorption cross section of the deuteron will deviate from the sum of the two absorption cross sections simply because one of its particles will sometimes lie in the shadow cast by the other. One has no trouble in correcting the absorption cross section since it is clear that the incident particle cannot be absorbed more than once. Let us say that the absorption cross sections of the neutron and proton are $\sigma_{n\text{abs}}$ and $\sigma_{p\text{abs}}$, respectively, and that their interaction radii are much smaller than the deuteron radius. Then to correct the absorption cross section for the deuteron we need only perform a simple geometrical calculation. The solid angle subtended by one particle as seen from the other, and the two configurations in which the correction is required, show us that the absorption cross section of the deuteron is

$$\sigma_{d\text{abs.}} = \sigma_{p\text{abs.}} + \sigma_{n\text{abs.}} - 2\sigma_{p\text{abs.}}\sigma_{n\text{abs.}} \left\langle \frac{1}{4\pi r^2} \right\rangle_d , \quad (174)$$

where in the correction term the inverse square of the neutron-proton distance is averaged in the deuteron ground state.

The correction to the absorption cross section comes from an effect which, as we have seen, is very close to a classical picture of an eclipse. The correction to the scattering cross section, however, is not at all so simple in its interpretation. There is quite a variety of effects which all contribute corrections of similar magnitudes. Such effects are: interference of single scattering amplitudes for the two particles, double scattering, interference of single and double scattering, and scattering by one particle followed by absorption by the other. These corrections are all significant but their separate consideration may be avoided by a simple stratagem.

At an earlier point we noted that, regardless of the shape of a black obstacle, its total cross section is twice its absorption cross section. That means that the total cross section of the deuteron may be obtained simply by multiplying Eq. (174) by two. In doing that we introduce the neutron and proton total cross sections $\sigma_n = 2\sigma_{n\text{abs}}$ and $\sigma_p = 2\sigma_{p\text{abs}}$ to find

$$\sigma_d = \sigma_n + \sigma_p - \frac{\sigma_n \sigma_p}{4\pi} \left\langle \frac{1}{r^2} \right\rangle_d . \quad (175)$$

Now this expression, simple as it is to derive, takes proper account of all the long list of corrections mentioned above, i.e., interference, etc. It furnishes an illustration of the advantage of treating interactions with the target system as a whole, wherever possible, rather than encounters between individual particles.

The correction term in Eq. (175) is indeed of the order of magnitude of the cross section differences observed. The proportionality of the

correction to the product of the total cross sections means that the effect becomes much more noticeable as the cross sections increase. A very large effect of this type must be present, for example, in antiproton-deuteron scattering, if the cross section of the free neutron is of the same order of magnitude as the rather large antiproton-proton cross section discovered recently. In that case analysis of the present sort becomes quite necessary in order to reach a reasonable estimate of the neutron cross section from a knowledge of the deuteron and proton cross sections. For the numbers actually observed in that case the indicated correction increases the estimated antiproton-neutron cross section by some forty to fifty per cent, and thereby shows it to be approximately as large as the antiproton-proton cross section.¹³

Since the effect we are considering occurs under a wide variety of conditions, and is not necessarily a small one, it is of interest to generalize the model we have used. We shall remove the assumptions that the nucleons are effectively black, and that the interaction ranges are much smaller than the deuteron radius. The latter, in fact, is a rather poor approximation.

Consider first the scattering of the incident particle by a single nucleon, say a neutron. The scattering amplitude is given by

$$f_n(\vec{k}', \vec{k}) = \frac{k}{2\pi i} \int e^{i(\vec{k}-\vec{k}') \cdot \vec{b}} \{ e^{i\chi_n(\vec{b})} - 1 \} d^{(a)} b. \quad (176)$$

Note that no account is taken of recoil, i.e., the neutron might as well be fixed. (For small-angle scattering, recoil corrections are proportional to θ^2 and hence are unimportant.) A similar expression yields the amplitude for scattering by the proton.

Now the amplitude for elastic scattering by the deuteron may, according to the results of the preceding section, be constructed as follows: Let \vec{q} be the neutron-proton separation, $\vec{q} = \vec{r}_n - \vec{r}_p$, and let $u(\vec{q})$ be the ground state wave function of a deuteron at rest. The projection of \vec{q} on the plane perpendicular to \vec{k} will be written as \vec{s} . Then the elastic scattering amplitude is

$$F(\vec{k}', \vec{k}) = \frac{k}{2\pi i} \int e^{i(\vec{k}-\vec{k}') \cdot \vec{b}} d^{(a)} b / |u(\vec{q})|^2 [e^{i\chi(\vec{b}, \vec{s})} - 1] d\vec{q} \quad (177)$$

where the phase shift $X(\vec{b}, \vec{s})$ is the sum of the phase shifts produced by the neutron and proton in their instantaneous positions,

$$X(\vec{b}, \vec{s}) = X_n(\vec{b} - \frac{\vec{s}}{2}) + X_p(\vec{b} + \frac{\vec{s}}{2}). \quad (178)$$

The scattering amplitudes are Fourier transforms of a set of functions which we may write as

$$\begin{aligned} \Gamma_n(\vec{b}) &= 1 - e^{iX_n(\vec{b})}, & \Gamma_p(\vec{b}) &= 1 - e^{iX_p(\vec{b})} \\ \Gamma(\vec{b}, \vec{s}) &= 1 - e^{i[X_n(\vec{b} - \frac{\vec{s}}{2}) + X_p(\vec{b} + \frac{\vec{s}}{2})]}. \end{aligned} \quad (179)$$

These functions vanish when \vec{b} lies outside the appropriate interaction ranges. Now, the last of these functions may be expressed in terms of the first two by means of the simple identity

$$\begin{aligned} \Gamma(\vec{b}, \vec{s}) &= 1 - [1 - \Gamma_n(\vec{b} - \frac{\vec{s}}{2})][1 - \Gamma_p(\vec{b} + \frac{\vec{s}}{2})] \\ &= \Gamma_n(\vec{b} - \frac{\vec{s}}{2}) + \Gamma_p(\vec{b} + \frac{\vec{s}}{2}) - \Gamma_n(\vec{b} - \frac{\vec{s}}{2})\Gamma_p(\vec{b} + \frac{\vec{s}}{2}). \end{aligned} \quad (180)$$

On substituting this expression into Eq. (177) and shifting the origin of the \vec{b} -plane in the first two integrals we express the elastic scattering amplitude in the form

$$\begin{aligned} F(\vec{k}', \vec{k}) &= f_n(\vec{k}', \vec{k}) \int e^{i(\vec{k} - \vec{k}') \cdot \frac{\vec{s}}{2}} |u(\vec{q})|^2 d\vec{q} + f_p(\vec{k}', \vec{k}) \int e^{i(\vec{k} - \vec{k}') \cdot \frac{\vec{s}}{2}} |u(\vec{q})|^2 d\vec{q} \\ &+ \frac{k}{2\pi i} \int e^{i(\vec{k} - \vec{k}') \cdot \vec{b}} d^m b / |u(\vec{q})|^2 \Gamma_n(\vec{b} - \frac{\vec{s}}{2}) \Gamma_p(\vec{b} + \frac{\vec{s}}{2}) d\vec{q}. \end{aligned} \quad (181)$$

This expression explicitly separates the effects of single and double scattering. The first two terms are the amplitudes for single scattering by each of the two target particles. The third term contributes only for deuteron configurations in which the incident particle can pass through the two regions of interaction surrounding the neutron and proton, i.e., it represents double scattering. Triple and higher order scattering does not occur in this calculation since the scattering is assumed to take place predominantly through small angles.

The elastic scattering amplitude in the forward direction is given by

$$F(\vec{k}, \vec{k}) = f_n(\vec{k}, \vec{k}) + f_p(\vec{k}, \vec{k}) + \frac{k}{2\pi i} \int |u(\vec{q})|^2 \Gamma_n(\vec{b} - \frac{\vec{q}}{2}) \Gamma_p(\vec{b} + \frac{\vec{q}}{2}) d^{(2)} b d\vec{q} , \quad (182)$$

and from this, by means of the optical theorem, we immediately find the total cross section,

$$\sigma_d = \sigma_n + \sigma_p - 2 \operatorname{Re} \int |u(\vec{q})|^2 \Gamma_n(\vec{b} - \frac{\vec{q}}{2}) \Gamma_p(\vec{b} + \frac{\vec{q}}{2}) d^{(2)} b d\vec{q} \quad (183)$$

The last term here is evidently the general expression for the cross section defect. To evaluate it accurately one must know the functions Γ , or equivalently, the phase shift functions for interactions with both the neutron and proton, as well as the deuteron wave function, particularly for small neutron-proton separations. Once again, in evaluating the total cross section we have implicitly summed over all the effects which decrease the incident beam strength. That means that corrections of all the types detailed earlier, i.e., interference, etc., are properly taken into account by Eq. (183).

To show the correspondence of this result with our earlier geometrical analysis, we have only to assume that the interaction ranges are small compared with the deuteron radius. In that case the correction term of Eq. (183) may be integrated approximately, so that we have

$$\sigma_d = \sigma_n + \sigma_p + \frac{4\pi}{k^2} \{ f_n(0) f_p(0) \} \left\langle \frac{1}{r^2} \right\rangle_d . \quad (184)$$

If the neutron and proton are simply absorptive, i. e., their phase shifts are purely imaginary, their scattering amplitudes become imaginary as well, so that an application of the optical theorem reduces Eq. (184) to Eq. (175). It should be noted that the condition that the phase shifts be imaginary may correspond to any degree of grayness so that the present calculation is much more general than that for the black-sphere model we began with. In practice the interaction radii of nucleons and mesons are not small enough compared with the deuteron size for Eq. (184) to furnish more than a crude estimate. The correct result may be found from the general expression (183) by taking the finite size of the interaction regions into account.

Stripping of High-Energy Deuterons

Another type of problem, one which involves the deuteron as a high-energy projectile may be treated by methods similar to those we have just presented. One of the earliest observations made with high-energy deuteron beams was of their decomposition on passing through a target into well collimated beams of neutrons and protons of approximately half the incident energy. These emerging nucleons were described by Serber¹⁴ as constituents of deuterons which had made grazing collisions with target nuclei and in which the other member, either a neutron or a proton, had been greatly deflected by a strongly inelastic collision.

If the target nucleus is represented schematically by a complex potential well (anticipating the results of the next section), the major difference between a deuteron-nucleus collision and the collisions we have treated, of an unspecified incident particle with the deuteron, lies in the frame of reference used. Formulae such as (177) for $F(\vec{k}, \vec{k})$ apply equally well to cases in which the deuteron is moving and the incident particle (i. e., a nucleus) assumes the role of a stationary target. The functions $u_i(q)$ and $u_f(q)$ still refer to the internal states of the deuteron, but $\vec{h}\vec{k}$ and $\vec{h}\vec{k}'$ become the initial and final momenta of the deuteron center of mass. This formulation of the stripping problem has been used, for example, to show that the deuteron may be dissociated in grazing encounters with nuclei in which neither the neutron nor the proton suffers any strong collision.¹⁵ In effect the deuteron is disintegrated simply by the diffraction of particles about the edge of the nucleus. A more detailed treatment of deuteron-nucleus collisions based on essentially the present method has been published by Akhieser and Sitenko.¹⁶

The Optical Model for Elastic Scattering

Let us apply the approximation procedure described in the earlier sections to the collision of an incident particle with a nucleus. The co-ordinates of the particles which inhabit the nucleus will be written as

$$\vec{q}_1, \vec{q}_2, \dots, \vec{q}_N .$$

Now if the nucleus is initially in the state i , the elastic scattering amplitude is

$$F_{ii}(\vec{k}', \vec{k}) = \frac{k}{2\pi i} \int e^{i(\vec{k}-\vec{k}') \cdot \vec{b}} d^{(2)} b . \quad (185)$$

$$\int |u_i(\vec{q}_1, \dots, \vec{q}_N)|^2 \{e^{iX(\vec{b}, \vec{s}_1, \dots, \vec{s}_N)} - 1\} \prod_{j=1}^N d\vec{q}_j ,$$

where the phase $X(\vec{b}, \vec{s}_1, \dots, \vec{s}_N)$ is the sum of the phase shifts contributed by the individual nucleons

$$X(\vec{b}, \vec{s}_1, \dots, \vec{s}_N) = \sum_{j=1}^N X_j(\vec{b} - \vec{s}_j) . \quad (186)$$

In the above formulae the \vec{s}_j are, as before, the components of the \vec{q}_j perpendicular to \vec{k} .

Now it is clear from a comparison of initial and final states that the nucleus plays a relatively passive role in elastic scattering. It is reasonable to ask, therefore, whether a totally inert model of the nucleus can be constructed which yields precisely the same elastic scattering. A way of constructing such a static model would be to find a potential well which scatters the incident particle in the way desired. This procedure, if feasible, would reduce at least this aspect of the many-body problem to the consideration of an effective one-body problem.

Now the procedure we have described is, in fact, quite simple to carry out, using the high-energy approximation. Instead of solving directly for an effective potential, however, we shall first work with phase shift functions. We have only to compare the general expression (185) for a nucleus as target with the expression

$$f(\vec{k}', \vec{k}) = \frac{k}{2\pi i} \int e^{i(\vec{k}-\vec{k}') \cdot \vec{b}} \{e^{iX(\vec{b})} - 1\} d^{(2)} b , \quad (187)$$

for the scattering by a static potential. We see immediately that if we let the static potential have a phase shift function

$$X_{\text{opt.}}(\vec{b})$$

given by

$$e^{iX_{\text{opt}}(\vec{b})} = \int |u_i(\vec{q}_1, \dots, \vec{q}_N)|^2 e^{i \sum_{j=1}^N X_j(\vec{b} - \vec{s}_j)} \prod_l d\vec{q}_l , \quad (188)$$

we secure the desired equality

$$f(\vec{k}', \vec{k}) = F_{il}(\vec{k}', \vec{k}) . \quad (189)$$

The relation defining $X_{\text{opt}}(\vec{b})$ may be abbreviated a bit by writing

$$e^{iX_{\text{opt}}(\vec{b})} = \langle e^{iX(\vec{b}, \vec{s}_1, \dots, \vec{s}_N)} \rangle_i , \quad (190)$$

where the phase shift $X(\vec{b}, \vec{s}_1, \dots, \vec{s}_N)$ is given by Eq.(186), and the brackets $\langle \rangle_i$ signify that an average is to be taken over all configurations of nucleons in the i -th state.

Now, as we mentioned earlier, as long as the interactions we are considering furnish a complete description of the problem, the phase shift produced by each of the nuclear particles will be real. Hence their sum, $X(\vec{b}, \vec{s}_1, \dots, \vec{s}_N)$ will be real as well. The expression (190) for the optical phase shift shows, however, that $X_{\text{opt}}(\vec{b})$ must, in general, be complex. Mathematically, this can be seen by noting that the values of

$$\exp[iX(\vec{b}, \vec{s}_1, \dots, \vec{s}_N)]$$

are unit vectors in the complex plane. An average taken over such unit vectors must have absolute magnitude less than or equal to unity. Furthermore, the case of equality would be realized only if $X(\vec{b}, \vec{s}_1, \dots, \vec{s}_N)$ were independent of the configuration of nuclear particles. Since no such independence holds in general, we have

$$|e^{iX_{\text{opt}}(\vec{b})}| < 1 . \quad (191)$$

i.e., the optical phase shift function $X_{\text{opt}}(\vec{b})$ has a positive (and, in

general, non-vanishing) imaginary part.

The physical interpretation of the imaginary part of $X_{\text{opt}}(\vec{b})$ is, of course, quite simple. Not all of the particles colliding with the actual nucleus undergo elastic scattering. Those which undergo inelastic collisions must be absent from the purely elastic scattering described by the optical model. The optical potential describes their removal in terms of an effective absorption. To see this in somewhat more detail we note that the exponential

$$\exp[iX(\vec{b}, \vec{s}_1, \dots, \vec{s}_N)]$$

is a unitary operator on the nuclear states

$$u_j(\vec{q}_1, \dots, \vec{q}_N),$$

and the expression (188) is one of its diagonal matrix elements. Such a diagonal matrix element must, in general, have absolute value less than unity simply because the state

$$e^{iX(\vec{b}, \vec{s}_1, \dots, \vec{s}_N)} u_i(\vec{q}_1, \dots, \vec{q}_N)$$

contains nuclear states other than the initial state u_i . These other components are the final states of inelastic scattering processes. To formulate the inequality more precisely, we use the relation

$$\begin{aligned} \sum_f | \langle u_f^* e^{iX(\vec{b}, \vec{s}_1, \dots, \vec{s}_N)} u_i \rangle \prod_j d\vec{q}_j \rangle |^2 &= \\ &= | e^{iX_{\text{opt}}(\vec{b})} |^2 + \sum_{f \neq i} | \langle u_f^* e^{iX(\vec{b}, \vec{s}_1, \dots, \vec{s}_N)} u_i \rangle \prod_j d\vec{q}_j \rangle |^2 \quad (192) \\ &= 1, \end{aligned}$$

which follows from the definition of a unitary operator, and the definition (188) of

$$\exp[iX_{\text{opt}}(\vec{b})].$$

From this relation we see once again

$$\left| e^{i\chi_{opt}(\vec{b})} \right| \leq 1.$$

(The case of equality arises only when $\chi(\vec{b}, \vec{s}_1, \dots, \vec{s}_N)$ is diagonal in the initial nuclear state and there are thus no inelastic transitions.)

A simple way of gaining insight into the structure of the optical model is to calculate the phase shift function $\chi_{opt}(\vec{b})$ as a series expansion in powers of $\chi(\vec{b}, \vec{s}_1, \dots, \vec{s}_N)$, i.e., we write

$$\begin{aligned} \chi_{opt}(\vec{b}) &= -i \log \left\langle e^{i\chi(\vec{b}, \vec{s}_1, \dots, \vec{s}_N)} \right\rangle_i \\ &= -i \log \left\{ 1 + i \langle \chi \rangle_i - \frac{1}{2} \langle \chi^2 \rangle_i + \dots \right\}, \end{aligned} \quad (193)$$

which yields

$$\begin{aligned} \chi_{opt}(\vec{b}) &= \langle \chi(\vec{b}, \vec{s}_1, \dots, \vec{s}_N) \rangle_i \\ &\quad + \frac{i}{2} \left\{ \langle \chi^2(\vec{b}, \vec{s}_1, \dots, \vec{s}_N) \rangle_i - \langle \chi(\vec{b}, \vec{s}_1, \dots, \vec{s}_N) \rangle_i^2 \right\} + \dots. \end{aligned} \quad (194)$$

To first order we see that the expression for $\chi_{opt}(\vec{b})$ is simply the average of the function $\chi(\vec{b}, \vec{s}_1, \dots, \vec{s}_N)$, i.e., the phase shift for any particular set of nucleon positions, averaged over all nuclear configurations. If the interaction takes place by means of ordinary potentials the first order term of χ_{opt} is evidently real. An imaginary part for χ_{opt} appears only as a second order perturbation since it is due to the possibility of nuclear excitation. The second order term of χ_{opt} is evidently purely absorptive (i.e., positive imaginary) in character, since it involves just the mean variance of the phase shift function. The fluctuation of the phase shift function arises simply from the fact that the nucleons of the target nucleus are not fixed in position. Indeed were the nucleons fixed in position, the imaginary part of χ_{opt} would vanish, in accord with the purely elastic nature of the scattering in that case.

The power series expansion of the expression (193) for $\chi_{opt}(\vec{b})$ is of a type which is well known in statistical theory. To develop its higher order terms we may write it as

$$\begin{aligned} iX_{\text{opt}}(\vec{b}) &= \log \langle e^{iX} \rangle_i \\ &= i \langle X \rangle_i + \log \langle e^{i(X - \langle X \rangle_i)} \rangle_i . \end{aligned} \quad (195)$$

Now the expansion in powers of a parameter λ of the function

$$\log \langle e^{i\lambda(X - \langle X \rangle_i)} \rangle_i$$

is easily obtained. Its coefficients are simple homogeneous polynomials in the various central moments of the function $X(\vec{b}, \vec{s}_1, \dots, \vec{s}_N)$. The expansion which we find for $X_{\text{opt}}(\vec{b})$ may be written as

$$iX_{\text{opt}}(\vec{b}) = \sum_{n=1}^{\infty} \frac{i^n}{n!} K_n(\vec{b}) , \quad (196)$$

where the $K_n(\vec{b})$ are given by

$$K_1(\vec{b}) = \langle X(\vec{b}, \vec{s}_1, \dots, \vec{s}_N) \rangle_i$$

$$K_2(\vec{b}) = \langle (X(\vec{b}, \vec{s}_1, \dots, \vec{s}_N) - \langle X(\vec{b}, \vec{s}_1, \dots, \vec{s}_N) \rangle_i)^2 \rangle_i$$

$$K_3(\vec{b}) = \langle (X - \langle X \rangle_i)^3 \rangle_i$$

$$K_4(\vec{b}) = \langle (X - \langle X \rangle_i)^4 \rangle_i - 3 \langle (X - \langle X \rangle_i)^2 \rangle_i^2 . \quad (197)$$

$$K_5(\vec{b}) = \langle (X - \langle X \rangle_i)^5 \rangle_i - 10 \langle (X - \langle X \rangle_i)^2 \rangle_i \langle (X - \langle X \rangle_i)^3 \rangle_i$$

$$\begin{aligned} K_6(\vec{b}) &= \langle (X - \langle X \rangle_i)^6 \rangle_i - 16 \langle (X - \langle X \rangle_i)^2 \rangle_i \langle (X - \langle X \rangle_i)^4 \rangle_i \\ &\quad - 10 \langle (X - \langle X \rangle_i)^3 \rangle_i^2 - 15 \langle (X - \langle X \rangle_i)^2 \rangle_i^3 \\ &\dots \end{aligned}$$

The coefficients K_n are the cumulants of the distribution function for $X(\vec{b}, \vec{s}_1, \dots, \vec{s}_N)$, or the semi-invariants of Thiele,¹⁷ as they are also known to statisticians.

Once the optical phase shift function $X_{opt}(\vec{b})$ has been evaluated either by means of the integral (188) for the series (196), it may be used in a number of ways to reduce the many-particle problem to one involving, in effect, only the incident particle. In particular the scattering and total cross sections are given in terms of $X_{opt}(\vec{b})$ by means of the single-particle formulae (96) and (98). That the latter formula holds for the total cross section follows from the generalized form of the optical theorem (167) which was shown to hold for collisions with bound particles. In that discussion of the optical theorem an expression (169) was written for the inelastic part of the total cross section which we may generalize to the case of many bound particles as

$$\sigma_{inelast.} = \int d^{(2)}b \left\{ 1 - \left| \int |U_i(\vec{q}_1, \dots, \vec{q}_N)|^2 e^{i \sum X_j(\vec{b} - \vec{s}_j) \prod d\vec{q}_j} \right|^2 \right\} . \quad (198)$$

This expression may be written in terms of $X_{opt}(b)$ as

$$\sigma_{inelast.} = \int d^{(2)}b \left\{ 1 - |e^{i X_{opt}(\vec{b})}|^2 \right\} ,$$

which is simply the absorption cross section (98) for the equivalent single particle problem. This observation illustrates the self-consistency of our formalism; particles which are described as absorbed in traversing a nucleus indeed account correctly for those which appear in the inelastic scattering.

Although we have illustrated the derivation of the function $X_{opt}(\vec{b})$ for the particular case of a many-particle nucleus it is well to bear in mind that the concepts used make no particular reference to the number of degrees of freedom involved. The scattering system need only be capable of a response which permits inelastic collisions. The effective phase shift function is equally well defined (and a great deal simpler to calculate) if the scatterer consists only of a single bound particle. It is also well defined for schematic models of the nucleus which ignore all but a few degrees of freedom. In discussing rotational states, for example, it is convenient to represent the nucleus as a homogeneous ellipsoid having only the Euler angles as degrees of freedom. The calculation of $X_{opt}(b)$ for such a system describes the effect of rotational inelasticity on the elastic scattering.

Solution for the Optical Potential

The optical model, as it is conventionally represented, replaces the actual interaction of an incident particle with the nucleus by an effective potential which is complex. In the preceding section, however, we have derived an optical representation of the nucleus on the basis of a complex effective phase shift function, $\chi_{opt}(\vec{b})$, which may be found from a knowledge of the force laws between particles and the nuclear ground state wave function. The two representations are clearly equivalent under conditions in which our approximations hold. An effective potential $V_{opt}(r)$ corresponds to a unique phase shift function $\chi_{opt}(\vec{b})$ and vice versa. In calculations making use of these approximations the phase shift function is usually the more useful of the two, but there is no difficulty in providing an explicit evaluation of the optical potential.

If the optical potential is assumed to be spherically symmetric ($V_{opt} = V_{opt}(|\vec{r}|)$), the effective phase shift function is related to it by means of the equation

$$\chi_{opt}(b) = - \frac{1}{\hbar v} \int_{-\infty}^{\infty} V_{opt}(\sqrt{b^2 + z^2}) dz , \quad (199)$$

or

$$\chi_{opt}(b) = - \frac{2}{\hbar v} \int_b^{\infty} \frac{V_{opt}(r) r dr}{\sqrt{r^2 - b^2}} . \quad (200)$$

If $\chi_{opt}(b)$ is regarded as known and $V_{opt}(r)$ as unknown, the latter relation becomes an Abel integral equation, a type which may be solved in elementary terms. The solution, in fact, is

$$V_{opt}(r) = \frac{\hbar v}{\pi} \frac{1}{r} \frac{d}{dr} \int_r^{\infty} \frac{\chi_{opt}(b) b db}{\sqrt{b^2 - r^2}} \quad (201)$$

This expression completes, in principle, the construction of the optical potential from a knowledge of the elementary interactions.

Relation of the Optical Potential to the Scattering Amplitudes (for a Simple Model)

The foregoing formalism may be illustrated in a simple way by considering an independent particle model of the nucleus. The effects of nucleon-nucleon correlations which such a model neglects will be considered explicitly in the next section. It will be helpful, therefore, to phrase the problem in general terms before introducing the simplifying features of the model.

We assume that the phase shift functions $\chi_j(b)$ which describe the

interaction of the incident particle with the individual target nucleons ($j = 1, \dots, N$) are known, and introduce the functions

$$\Gamma_j(\vec{b}) = 1 - e^{i X_j(\vec{b})}. \quad (202)$$

These functions vanish for \vec{b} outside the nuclear force range. The scattering amplitude of the incident particle by the l -th nucleon, if it were isolated from the others ($j \neq l$), would be

$$f_l(\vec{k}', \vec{k}) = \frac{i k}{2\pi} \int e^{i(\vec{k}-\vec{k}') \cdot \vec{b}} \Gamma_l(\vec{b}) d^3 b. \quad (203)$$

We are, however, dealing with a situation in which multiple scattering involving all of the particles occurs. Once again we let \vec{q}_j be the nucleon coordinates and \vec{s}_j their projections on a plane perpendicular to the momentum of the incident particle. Now if we let $u_i(\vec{q}_1, \dots, \vec{q}_N)$ be the nuclear ground state wave function and make use of the identity

$$e^{i \sum_j X_j(\vec{b} - \vec{s}_j)} = \prod_{j=1}^N (1 - \Gamma_j(\vec{b} - \vec{s}_j)), \quad (204)$$

we may write the elastic scattering amplitude of the nucleus as

$$F_{ii}(\vec{k}', \vec{k}) = \frac{k}{2\pi i} \int e^{i(\vec{k}-\vec{k}') \cdot \vec{b}} \left\{ / |u_i(\vec{q}_1, \dots, \vec{q}_N)|^2 \prod_j (1 - \Gamma_j(\vec{b} - \vec{s}_j)) d\vec{q}_j - / \right\} d^3 b. \quad (205)$$

This expression is, in effect, simply an extension of Eqs. (177) and (181), for the scattering amplitude of the deuteron, to the case of a many-particle system. The product (204) may be expanded to the form

$$\prod_{j=1}^N (1 - \Gamma_j) = 1 - \sum_j \Gamma_j + \sum_{j \neq l} \Gamma_j \Gamma_l - \dots + (-1)^N \prod_{j=1}^N \Gamma_j . \quad (206)$$

When this expansion is substituted in Eq. (205), the terms containing a single function Γ_j may be expressed immediately in terms of the scattering amplitudes (203). If all further terms were dropped, the sum of these terms linear in the Γ_j would constitute the familiar single-scattering approximation

$$F_i(\vec{k}', \vec{k}) \approx \sum_{j=1}^N f_j(\vec{k}, \vec{k}') / e^{i(\vec{k}-\vec{k}') \cdot \vec{s}_j} |u_i(\vec{q}_1, \dots, \vec{q}_N)|^2 \prod_j d\vec{q}_j . \quad (207)$$

The further terms of the expansion (206) provide corrections for effects of multiple scattering and interference which become important in configurations in which nucleons lie in the "shadows" cast by one another.

The integrations required to find the nuclear scattering amplitude are simplified considerably by using an independent particle model for the nucleus. We assume, as a first approximation, that the nuclear ground state wave function factorizes so that $|u_i(\vec{q}_1, \dots, \vec{q}_N)|^2$ may be written as

$$|u_i(\vec{q}_1, \dots, \vec{q}_N)|^2 = \prod_j \rho_j(\vec{q}_j) , \quad (208)$$

where $\rho_j(\vec{q}_j)$ is the normalized density for the j -th particle. The integral (188) which defines the effective phase shift function is then given by

$$\begin{aligned} e^{i X_{opt}(\vec{b})} &= \int |u_i(\vec{q}_1, \dots, \vec{q}_N)|^2 \prod_{j=1}^N (1 - \Gamma_j(\vec{b} - \vec{s}_j)) d\vec{q}_j \\ &= \prod_{j=1}^N \left\{ 1 - \int \rho_j(\vec{q}_j) \Gamma_j(\vec{b} - \vec{s}_j) d\vec{q}_j \right\} . \end{aligned} \quad (209)$$

The function $\chi_{\text{opt}}(\vec{b})$ is thus given by

$$\chi_{\text{opt}}(\vec{b}) = -i \sum_j \log \left\{ 1 - \int \rho_j(\vec{q}_j) \Gamma_j(\vec{b} - \vec{s}_j) d\vec{q}_j \right\}, \quad (210)$$

where in each term the branch of the logarithm which approaches zero as $b \rightarrow \infty$ is to be chosen.

A further simplification which is convenient at this point is the assumption that the range a of the interactions between the incident particle and the target nucleons is much smaller than the nuclear radius R . In that case, since the functions Γ_j assume values at most of order unity within the force range and vanish outside it, the integrals

$$\int \rho_j(\vec{q}_j) \Gamma_j(\vec{b} - \vec{s}_j) d\vec{q}_j \quad (211)$$

must be quite small in absolute value. In fact they must vanish for values of b appreciably larger than R , and for smaller b take on values at most of order a^2/R^2 . We may therefore expand the arguments of the logarithms in (210) to find

$$\chi_{\text{opt.}}(\vec{b}) = i \sum_j \int \rho_j(\vec{q}_j) \Gamma_j(\vec{b} - \vec{s}_j) d\vec{q}_j + \dots \quad (212)$$

The higher order terms, which have been dropped for simplicity are at most of order a^2/R^2 relative to those retained.

Since there are only two types of nucleons within the nucleus, neutrons and protons, only two different functions Γ_j actually enter the problem. We shall carry the simplification one stage further, however, by assuming only one kind of particle to be present in the model nucleus. The actual case may be described by a self-evident extension of the notation.

If all the functions $\Gamma_j(b)$ take the same form, $\Gamma(b)$, the expression (212) for $\chi_{\text{opt}}(b)$ may be written in terms of the average particle density

$$\rho(\vec{q}) = \frac{1}{N} \sum_{j=1}^N \rho_j(\vec{q}) \quad (213)$$

as

$$\chi_{\text{opt}}(\vec{b}) = i N \int \rho(\vec{q}) \Gamma(\vec{b} - \vec{s}) d\vec{q}. \quad (214)$$

The average density function $\rho(\vec{q})$ presumably varies fairly smoothly over the nuclear volume. We may therefore take advantage once more of the smallness of the force range to carry out the integration (214) in an approximate way. For this purpose it is convenient to write the argument of the function $\rho(\vec{q})$ in terms of its components z , parallel to \vec{k} , and \vec{s} , perpendicular to \vec{k} , i.e.,

$$\rho(\vec{q}) = \rho(\vec{s}, z).$$

We then find, again by neglecting terms of relative order a^2/R^2 ,

$$\chi_{opt}(\vec{b}) = i N \int \Gamma(\vec{s}) d^{(2)} \vec{s} \int_{-\infty}^{\infty} \rho(\vec{b}, z) dz. \quad (215)$$

Now, according to Eq. (203), the amplitude for forward scattering by a single nucleon is

$$f(0) = \frac{ik}{2\pi} \int \Gamma(\vec{b}) d^{(2)} b. \quad (216)$$

Hence the effective phase shift function may be written as

$$\chi_{opt}(\vec{b}) = \frac{2\pi N}{k} f(0) \int \rho(\vec{b}, z) dz. \quad (217)$$

Since the function ρ is, in general, spherically symmetric, it is clear that this phase shift function corresponds to an optical potential which has the same form as the density. The optical potential is given by

$$\begin{aligned} -\frac{1}{\hbar v} V_{opt}(r) &= \frac{2\pi N}{k} f(0) \rho(r) \\ &= N \left[\frac{2\pi}{k} R e f(0) + \frac{i}{2} \sigma \right] \rho(r), \end{aligned} \quad (218)$$

where σ is the total cross section of a single nucleon. An equivalent description of the scattering may be made in terms of a complex nuclear refractive index $n(r)$ given by

$$n(r) - 1 = \frac{2\pi N}{k^2} f(0) \rho(r). \quad (219)$$

This is an expression frequently quoted in the literature, but rarely with much indication of the conditions under which it holds. The present derivation besides requiring conditions favorable to the high energy approximation, has assumed the nucleons to move independently of one another and has neglected terms of order a^2/R^2 .

The foregoing considerations are easily generalized to include spin-orbit interactions between the incident particle and the target nucleons. The functions $\Gamma(b)$, which we assume for simplicity remain the same for all nucleons, are then given by

$$\Gamma(\vec{b}) = \Gamma_c(\vec{b}) + i \vec{\sigma} \cdot \left(\frac{\vec{b}}{b} \times \hat{R} \right) \Gamma_s(\vec{b}), \quad (220)$$

where Γ_c and Γ_s are the axially symmetric functions defined by (131) and (132). The optical phase shift function may be evaluated as before by substituting this expression in (214) and approximating the required integral. The treatment of the non-spin-dependent term to order a^2/R^2 is the same as in the previous case. The spin-dependent term, however, requires a bit more attention. To the extent that the function

$$\int_{-\infty}^{\infty} \rho(\vec{s}, z) dz$$

may be regarded as a constant independent of \vec{s} within the nucleon interaction range, the integral of the spin-dependent term vanishes. To evaluate this term, therefore, the function

$$\int_{-\infty}^{\infty} \rho(\vec{s}, z) dz$$

must be expanded in a power series about the point $\vec{s} = \vec{b}$, i.e., by introducing the vector $\vec{l} = \vec{b} - \vec{s}$ we may write

$$\begin{aligned} \int \rho(\vec{q}) \Gamma(\vec{b} - \vec{s}) d\vec{q} &= \\ \int \rho(\vec{b} - \vec{l}, z) \left\{ \Gamma_c(\vec{l}) + i \vec{\sigma} \cdot \left(\frac{\vec{l}}{l} \times \hat{R} \right) \Gamma_s(\vec{l}) \right\} d^{(2)}l dz \\ &\approx \int \Gamma_c(\vec{l}) d^{(2)}l \int_{-\infty}^{\infty} \rho(\vec{b}, z) dz + \\ &\quad i \vec{\sigma} \cdot \left[\hat{R} \times \int \frac{1}{l} \Gamma_s(l) \vec{l} \cdot \nabla_b \int_{-\infty}^{\infty} \rho(\vec{b}, z) dz d^{(2)}l \right]. \end{aligned} \quad (221)$$

If the spin-orbit and central forces are of comparable magnitudes the spin-dependent term above is smaller than the spin-independent one by a factor of order a/R . Although spin-dependence must therefore be viewed as a small effect it may be consistently retained in an expansion which neglects terms of order a^2/R^2 .

The integrals of the functions Γ_c and Γ_s which occur in (221) may be related to the two terms $f(\vec{k}, \vec{K})$ and $g(\vec{k}, \vec{K})$ of the spin-dependent scattering amplitude of a nucleon defined by (135) and (136). Clearly the integral of Γ_c is related to the forward value of the spin-independent amplitude f ,

$$f(0) = f(\vec{k}, \vec{k}) = \frac{i\vec{k}}{2\pi} \int \Gamma_c(\vec{b}) d^{(2)}b. \quad (222)$$

Advantage may be taken of the axial symmetry of the function Γ_s by writing the integral involving it as

$$\int \frac{l_i l_j}{l} \Gamma_s(l) d^{(2)}l = \frac{1}{2} \delta_{ij} \int l \Gamma_s(l) d^{(2)}l, \quad (223)$$

where the indices i and j label cartesian axes. The latter integral may be expressed in terms of the derivative with respect to the scattering angle ϑ of the spin-dependent amplitude g near the forward direction

$$\begin{aligned} \frac{1}{2} \int b \Gamma_s(b) d^{(2)}b &= \frac{2\pi i}{k^2} \frac{d}{d\vartheta} g(\vartheta) \Big|_{\vartheta=0} \\ &= \frac{2\pi i}{k^2} g'(0). \end{aligned} \quad (224)$$

Hence, with the presence of a spin-orbit interaction, we find the effective phase shift function

$$\begin{aligned} \chi_{\text{opt}}(\vec{b}) &= iN \int \rho(\vec{q}) \Gamma(\vec{b} - \vec{s}) d\vec{q} \\ &= \frac{2\pi N}{k} \left\{ f(0) - \frac{i}{k} g'(0) \vec{\sigma} \cdot (\vec{K} \times \nabla_b) \right\}_{-\infty}^{\infty} \rho(b_z) dz. \end{aligned} \quad (225)$$

An optical potential may be derived from this expression by writing it in the equivalent form

$$\chi_{\text{opt}}(\vec{b}) = \quad \quad \quad (226)$$

$$\frac{2\pi N}{k} \int \left\{ f(o) - \frac{i}{k} g'(o) \vec{\sigma} \cdot (\hat{R} \times \nabla_q) \right\} \rho(\vec{q}) dz \Big|_{\vec{q} - R(\vec{R} \cdot \vec{q}) = \vec{b}} .$$

This form makes it evident that a suitable potential is given by

$$-\frac{1}{hv} V_{\text{opt}}(\vec{r}) = \frac{2\pi N}{k} \left\{ f(o) - \frac{i}{k} g'(o) \vec{\sigma} \cdot (\hat{R} \times \nabla_r) \right\} \rho(r). \quad (227)$$

Since the average density function is spherically symmetric we have

$$\nabla_r \rho(r) = \vec{F} \frac{d}{dr} \rho(r) .$$

We must now remember that \hat{K} is a unit vector in the direction of the incident momentum $\hbar \vec{K}$ (or, the nearly parallel direction given by (89)). The vector product $(\vec{F} \times \vec{K})$ is of course the orbital angular momentum (in units of \hbar) of the incident particle. Hence the optical potential takes a form such that

$$-\frac{1}{hv} V_{\text{opt}}(r) = \frac{2\pi N}{k} \left\{ f(o) \rho(r) + \frac{i}{k} g'(o) \frac{1}{r} \frac{d}{dr} \rho(r) \vec{\sigma} \cdot \vec{L} \right\} . \quad (228)$$

It is of considerable interest to note that the spin-orbit portion of this potential falls naturally into a form bearing an analogy to the Thomas interaction of atomic theory. Such a form was employed by Fermi in an early analysis of polarization experiments, and has been widely used since. We have shown that this form follows naturally from a power series expansion in the ratio a/R . Furthermore the coefficient of the spin-orbit potential, $(i/k^2)g'(o)$, is complex and may be established directly from suitable scattering and polarization measurements on single-nucleon targets.

The expression (228) for the optical spin-orbit potential is not an unfamiliar one, but previous derivations of it appear to have been confined to the single-scattering approximation analogous to (207). Such derivations, of course, do not justify the use of the potential (228) in calculations to any accuracy higher than the first order of perturbation theory. The actual discussion of polarization experiments, however, has required

a much more accurate treatment than perturbation theory, and hence the implicit assumption that the interaction (228) is correct to higher order as well. The present derivation, by implicitly summing the effects of multiple scattering, goes considerably further to justify the use of this interaction in the high-energy limit. The particular form found for the spin-orbit interaction depends on the assumption that the force range is much smaller than the nuclear radius.

Where this is not so, as in the α particle, for example, the spin-orbit potential may assume a rather different shape. A key point in the derivation has been the assumption that the nucleons are uncorrelated in position within the nucleus. The presence of correlations introduces corrections to the optical potential which we shall discuss in the next section.

Influence of Nucleon Correlations on the Optical Model

18

Various types of correlations in position and spin may exist between the nucleons of an actual nucleus. Attractive or repulsive forces between the particles will in general lead to such deviations from independent-particle behavior, but correlations must be expected even in the absence of interaction effects. A certain correlation is introduced simply by the circumstance that nucleons are Fermi particles. This may be seen from the fact that an antisymmetric wave function vanishes whenever two similar particles have the same space and spin coordinates.

All of the information we require about the correlations is contained, of course, in the square of the absolute value of the nuclear ground state wave function, $u_i(\vec{q}_1, \dots, \vec{q}_N)$. To develop a more convenient notation we shall define an N -particle density function $\rho^{(N)}(\vec{q}_1, \dots, \vec{q}_N)$ as

$$\rho^{(N)}(\vec{q}_1, \dots, \vec{q}_N) = |u_i(\vec{q}_1, \dots, \vec{q}_N)|^2, \quad (229)$$

which is symmetric in its N variables. A succession of density functions involving $N-1$, $N-2, \dots$ coordinates may be defined by integrating over the remaining coordinates

$$\begin{aligned} \rho^{(N-1)}(\vec{q}_1, \dots, \vec{q}_{N-1}) &= \int \rho^{(N)}(\vec{q}_1, \dots, \vec{q}_N) d\vec{q}_N \\ \dots \\ \rho^{(2)}(\vec{q}_1, \vec{q}_2) &= \int \rho^{(3)}(\vec{q}_1, \vec{q}_2, \vec{q}_3) d\vec{q}_3 \\ \rho^{(1)}(\vec{q}_1) \equiv \rho(\vec{q}_1) &= \int \rho^{(2)}(\vec{q}_1, \vec{q}_2) d\vec{q}_2 . \end{aligned} \quad (230)$$

Each of these functions is symmetric and normalized to unity when inte-

grated over all of its coordinates. The symbol ϱ is introduced as an abbreviation for $\varrho^{(n)}$. This function will be seen to play the same role as the independent-particle density ϱ of the preceding section.

According to the definition (188), the optical phase shift function may be expressed in the form

$$\begin{aligned} \chi_{\text{opt}}(\vec{b}) &= -i \log \int \rho^{(n)}(\vec{q}_1, \dots, \vec{q}_N) e^{i \sum_j \chi_j(\vec{b} - \vec{s}_j)} \prod_j d\vec{q}_j \\ &= -i \log \left\langle e^{i \sum_j \chi_j(\vec{b} - \vec{s}_j)} \right\rangle_i . \end{aligned} \quad (231)$$

If we again introduce the functions Γ , according to (204), and assume all the nucleons identical, we have

$$\chi_{\text{opt}}(\vec{b}) = -i \log \left\langle \prod_{j=1}^N (1 - \Gamma(\vec{b} - \vec{s}_j)) \right\rangle_i . \quad (232)$$

To illustrate a way in which this expression may be evaluated, it is convenient to simplify the notation a bit and introduce a certain parametric dependence on a new variable λ . Let us consider the function

$$\mathcal{L}(\lambda) = \log \left\langle \prod_j (1 + \lambda S(q_j)) \right\rangle , \quad (233)$$

where the function $S(q_j)$ obviously plays the role of $-\Gamma(b - s_j)$ in (232). We now expand the function $\mathcal{L}(\lambda)$ in a power series about $\lambda = 0$.

$$\mathcal{L}(0) = 0 , \quad (234)$$

$$\begin{aligned} \frac{d\mathcal{L}}{d\lambda} \Big|_{\lambda=0} &= \frac{\sum_i \left\langle S(q_i) \prod_{j \neq i} (1 + \lambda S(q_j)) \right\rangle}{\left\langle \prod_j (1 + \lambda S(q_j)) \right\rangle} \Big|_{\lambda=0} = \sum_i \left\langle S(q_i) \right\rangle \\ &= N \left\langle S(q_1) \right\rangle = N / S(\vec{q}) \varrho(\vec{q}) d\vec{q} , \end{aligned} \quad (235)$$

$$\begin{aligned}
 \left. \frac{d^2\mathcal{L}}{d\lambda^2} \right|_{\lambda=0} &= \left[\frac{\sum_{i \neq k} \langle S(q_i) S(q_k) \prod_{j \neq i, k} (1 + \lambda S(q_j)) \rangle}{\langle \prod_j (1 + \lambda S(q_j)) \rangle} \right. \\
 &\quad \left. - \frac{\sum_{i, k} \langle S(q_i) \prod_{j \neq i} (1 + \lambda S(q_j)) \rangle \langle S(q_k) \prod_{j \neq k} (1 + \lambda S(q_j)) \rangle}{\langle \prod_j (1 + \lambda S(q_j)) \rangle^2} \right]_{\lambda=0} \quad (236) \\
 &= \sum_{i \neq k} \langle S(q_i) S(q_k) \rangle - \sum_{i, k} \langle S(q_i) \rangle \langle S(q_k) \rangle \\
 &= N(N-1) \langle S(q_1) S(q_2) \rangle - N^2 \langle S(q_1) \rangle^2 \\
 &= \int S(\vec{q}_1) S(\vec{q}_2) \{ N(N-1) \rho^{(2)}(\vec{q}_1, \vec{q}_2) - N^2 \rho(\vec{q}_1) \rho(\vec{q}_2) \} d\vec{q}_1 d\vec{q}_2 .
 \end{aligned}$$

$$\left. \frac{d^3\mathcal{L}}{d\lambda^3} \right|_{\lambda=0} = \int S(\vec{q}_1) S(\vec{q}_2) S(\vec{q}_3) \{ N(N-1)(N-2) \rho^{(3)}(\vec{q}_1, \vec{q}_2, \vec{q}_3) - \right. \\
 \left. 3N^2(N-1) \rho^{(2)}(\vec{q}_1, \vec{q}_2) \rho(\vec{q}_3) + 2N^3 \rho(\vec{q}_1) \rho(\vec{q}_2) \rho(\vec{q}_3) \} d\vec{q}_1 d\vec{q}_2 d\vec{q}_3 . \quad (237)$$

These averages may be expressed a bit more briefly in terms of the actual particle densities, which may be written as

$$\begin{aligned}
 n(\vec{q}) &= N \rho(\vec{q}) \quad , \quad n^{(2)}(\vec{q}_1, \vec{q}_2) = N(N-1) \rho^{(2)}(\vec{q}_1, \vec{q}_2) , \dots \\
 n^{(r)}(\vec{q}_1, \dots, \vec{q}_r) &= \frac{N!}{(N-r)!} \rho^{(r)}(\vec{q}_1, \dots, \vec{q}_r) .
 \end{aligned} \quad (238)$$

The expansion of $\mathcal{L}(\lambda)$ is then

$$\begin{aligned}
 \mathcal{L}(\lambda) &= \lambda \int S(q) n(q) dq + \\
 &\quad \frac{\lambda^2}{2} \int S(q_1) S(q_2) \{ n^{(2)}(q_1, q_2) - n(q_1) n(q_2) \} dq_1 dq_2 + \dots . \quad (239)
 \end{aligned}$$

The expression (232) for the optical phase shift function may be evaluated by means of the expansion (239) by substituting $S(\vec{q}_1) = -\Gamma(\vec{b} - \vec{s}_1)$ and $\lambda = 1$. The phase shift function is then found to be

$$\begin{aligned} \chi_{\text{opt.}}(\vec{b}) = & i \int n(\vec{q}) \Gamma(\vec{b} - \vec{s}) d\vec{q} \\ & - \frac{i}{2} \int [n^{(2)}(\vec{q}_1, \vec{q}_2) - n(\vec{q}_1)n(\vec{q}_2)] \Gamma(\vec{b} - \vec{s}_1) \Gamma(\vec{b} - \vec{s}_2) d\vec{q}_1 d\vec{q}_2 \\ & + \frac{i}{6} \int [n^{(3)}(\vec{q}_1, \vec{q}_2, \vec{q}_3) - 3n^{(2)}(\vec{q}_1, \vec{q}_2)n(\vec{q}_3) + \\ & 2n(\vec{q}_1)n(\vec{q}_2)n(\vec{q}_3)] \Gamma(\vec{b} - \vec{s}_1) \Gamma(\vec{b} - \vec{s}_2) \Gamma(\vec{b} - \vec{s}_3) d\vec{q}_1 d\vec{q}_2 d\vec{q}_3 + \dots \end{aligned} \quad (240)$$

The first term of this expansion is of precisely the form discussed in the preceding section. The function $n(\vec{q}) = N\rho(\vec{q})$ plays in it the same role as the density in the independent-particle model. The succeeding terms of the expansion represent the effects of pair correlations, three-particle correlations, etc. To illustrate these effects further we shall discuss the second term of the series in a simple limit.

If the number of particles, N , is quite large, it becomes convenient to write the two-particle density $n^{(2)}$ in the form

$$n^{(2)}(\vec{q}_1, \vec{q}_2) = n(\vec{q}_1)n(\vec{q}_2) \left\{ g(\vec{q}_1, \vec{q}_2) + \frac{h(\vec{q}_1, \vec{q}_2)}{N} + O\left(\frac{1}{N^2}\right) \right\}. \quad (241)$$

An expression of this type is useful since the function $n^{(2)}(\vec{q}_1, \vec{q}_2)$ will not in general deviate appreciably from the product $n(\vec{q}_1)n(\vec{q}_2)$ unless the points \vec{q}_1 and \vec{q}_2 are fairly close together. The function $h(\vec{q}_1, \vec{q}_2)/N$ is added within the parentheses so that the pair density function $g(\vec{r}, \vec{r}')$ may be defined to take on the asymptotic value unity as either \vec{r} or \vec{r}' recedes to infinity. The function h takes on values of order unity and so the correction h/N may be neglected in integrals over small volumes. If the system being considered is spatially uniform, the pair density $g(\vec{r}, \vec{r}')$ will depend only on the distance $|\vec{r} - \vec{r}'|$. With this assumption we may write

$$n^{(2)}(\vec{q}_1, \vec{q}_2) - n(\vec{q}_1)n(\vec{q}_2) \approx n(\vec{q}_1)n(\vec{q}_2) \{g(|\vec{q}_1 - \vec{q}_2|) - 1\} \quad (242)$$

An idea of the magnitude and nature of the effects due to pair correlations may be obtained by assuming once again that the interaction range of a nucleon is small. In this limit the second term of the expansion (240) may be approximated as

$$\begin{aligned} & -\frac{i}{2} \int [n^{(2)}(\vec{q}_1, \vec{q}_2) - n(\vec{q}_1)n(\vec{q}_2)] \Gamma(\vec{b}-\vec{s}_1)\Gamma(\vec{b}-\vec{s}_2) d\vec{q}_1 d\vec{q}_2 \\ & \approx -\frac{i}{2} \left(\frac{2\pi}{ik} f(0) \right)^2 \int_{-\infty}^{\infty} n^2(\vec{b}, z) dz \cdot 2 \int_0^{\infty} [g(|r|) - 1] dr , \end{aligned} \quad (243)$$

where the notation $n(\vec{s}, z) = n(\vec{q})$ has been used. The pair density function $g(|r|)$ is defined to approach unity as $|\vec{r}| \rightarrow \infty$. The distance within which $g-1$ undergoes a substantial decrease may be termed the correlation length ℓ . It should be noted that the expression (243) is based on the assumption that this distance considerably exceeds the range of nucleon-nucleon forces, i.e., $\ell \gg a$. Furthermore the assumption of homogeneity which makes g a function of a single distance requires that ℓ be much smaller than the nuclear radius R . Because R is not vastly larger than a , these conditions cannot both be satisfied very well for actual nuclei. Since the correlation length is not too different in magnitude from the force range, the short-range approximation (243) should only be used for rough estimates.

When the short-range approximation is used the expression (240) for the optical phase shift becomes

$$\begin{aligned} \chi_{opt}(\vec{b}) &= \frac{2\pi}{k} f(0) \int_{-\infty}^{\infty} n(\vec{b}, z) dz + \\ & i \left(\frac{2\pi}{k} f(0) \right)^2 \int_0^{\infty} [g(|r|) - 1] dr \int_{-\infty}^{\infty} n^2(\vec{b}, z) dz + \dots \end{aligned} \quad (244)$$

This form for the phase shift function is evidently equivalent to an optical potential given by

$$\begin{aligned} -\frac{1}{\hbar v} V_{opt}(r) &= \frac{2\pi N}{k} f(0) \rho(r) + \\ & i \left(\frac{2\pi N}{k} f(0) \right)^2 \rho^2(r) \int_0^{\infty} [g(|r|) - 1] dr + \dots \end{aligned} \quad (245)$$

The first term of this expansion is of a form we have already encountered in discussing the independent-particle model. The succeeding terms,

which represent the effects of nucleon-nucleon correlations, correspond to an expansion of the optical potential in powers of the nucleon density. The series is equally well an expansion in powers of the forward scattering amplitude; it possesses the dimensionless expansion parameter $2\pi\lambda f(\omega)n$.

Since the forward scattering amplitude $f(\omega)$ is complex, the correlation term in (245) corrects both the real and imaginary parts of the optical potential. By using the optical theorem these parts may be written as

$$-\frac{1}{\hbar v} \operatorname{Re} V_{\text{opt.}}(r) = \frac{2\pi}{k} n(r) \operatorname{Re} f(\omega) \left\{ 1 - \sigma n(r) \int_r^\infty (g(r) - 1) dr \right\} \quad (246)$$

$$-\frac{1}{\hbar v} \operatorname{Im} V_{\text{opt.}}(r) = n(r) \frac{1}{2} \left\{ \sigma + \frac{8\pi^2}{k^2} [(\operatorname{Re} f(\omega))^2 - (\operatorname{Im} f(\omega))^2] n(r) \int_r^\infty (g(r) - 1) dr \right\} \quad (247)$$

$$= n(r) \frac{1}{2} \left\{ \sigma + \frac{1}{2} \left[\left(\frac{4\pi}{k} \operatorname{Re} f(\omega) \right)^2 - \sigma^2 \right] n(r) \int_r^\infty (g(r) - 1) dr \right\}.$$

The correction terms due to correlations are not necessarily small in magnitude. If, for example, the correlation length is $\lambda = 2 \times 10^{-13}$ cm, the total cross section of an isolated nucleon is $\sigma = 40$ millibarns, and the particle density is that of actual nuclei, the correction to the real part of the optical potential may be of the same magnitude as the independent-particle term. Larger cross sections, such as occur for incident antiprotons, will tend proportionally to increase the correction. Other factors, however, will tend to diminish the correlation effect to some extent. Correlations which keep particles apart, such as those due to repulsive forces and the exclusion principle, lead to negative values of the function $g(r) - 1$. Any attractive correlations present will tend to compensate the repulsive ones by leading to positive values of $g(r) - 1$. The correlations of actual nucleons may be expected to depend considerably on their spin and charge states. A further consideration which tends to diminish the correlation effect somewhat is the removal of the short-range approximation for the force between the incident particle and the nucleons. This approximation overestimates the corrections due to nucleons which lie at distances apart smaller than the force range.

The technique we have used in discussing correlations may easily be extended in various directions. We may, for example, seek the effect of correlations in the presence of spin-orbit forces. Since the functions $\Gamma(\vec{s}_i - \vec{s}_j)$ are operators in this case, and the particle density no longer

factorizes, it is necessary to pay careful attention to the ordering of factors. The result is simplest to state for the case in which the correlation length is much smaller than the nuclear radius. It is

$$\begin{aligned} -\frac{1}{\hbar v} V_{\text{opt}}(r) &= \frac{2\pi}{k} \left\{ f(0)n(r) + \frac{i}{k^2} g'(0) \frac{1}{r} \frac{d}{dr} n(r) \vec{\sigma} \cdot \vec{L} \right\} \\ &\quad + i \left(\frac{2\pi}{k} \right)^2 n^2(r) \left\{ f^2(0) \int_0^\infty (q(r)-1) dr + \left(\frac{g'(0)}{k} \right)^2 \int_0^\infty \frac{2}{r} \frac{d}{dr} q(r) dr \right\}. \end{aligned} \quad (248)$$

The function $g'(0)$ which appears here is the derivative of the spin-dependent scattering amplitude (224) evaluated for $\vec{\sigma} = 0$. The function $g(r)$ occurring in the integrands is again the pair density, defined by (241). The correlation term in (248) has been evaluated under the assumption that the nucleon density varies very slowly within a correlation length. The contributions from the nuclear surface which are thereby neglected may easily be constructed by the same means. The short-range approximation $a \ll l$ has also been used in deriving (248).

The Influence of the Exclusion Principle on the Optical Potential

The constraint of antisymmetry which the exclusion principle places upon a nuclear wave function produces certain correlations in the positions of the individual nucleons. The most important consequences of the exclusion principle may be described in terms of these correlations; their effects are present whatever is the nature of the incident particle.

We may assume, for the moment, in order to separate two problems, that the incident particle is not a nucleon. Then our main task in estimating the correlation effect is the evaluation of the pair density function $g(r)$. For the simple model of a gas of many non-interacting Fermi particles, this function may be evaluated quite readily. Its derivation is usually discussed in connection with treatments of the electron gas in conductors. We define the Fermi momentum k_F via the relation

$$\frac{1}{6\pi^2} k_F^3 = n, \quad (249)$$

where n is the density of nucleons (of similar charge and spin variables). Then the pair density function may be written as

$$\begin{aligned} g(r) &= 1 - \frac{9\pi}{2} \frac{1}{(k_F r)^3} [J_{3/2}(k_F r)]^2 \\ &= 1 - q \left\{ \frac{\sin k_F r - k_F r \cos k_F r}{k_F^3 r^3} \right\}^2. \end{aligned} \quad (250)$$

The pair density (250) may be seen to vanish for $r = 0$, and to approach unity for distances large compared to the Fermi wavelength, $1/k_F$. This behavior expresses the tendency of fermions of similar charge and spin to remain separated from one another; i.e., their positions are anticorrelated.

To evaluate the correlation effect in the short-range approximation we require the integral

$$\int_0^\infty (g(r) - 1) dr = - \frac{q\pi}{2k_F} \int_0^\infty \frac{1}{x^3} (J_{3/2}(x))^2 dx \\ = - \frac{3\pi}{5k_F} . \quad (251)$$

By using the definition, (249), of the Fermi momentum we may write

$$n(r) \int_0^\infty (g(r) - 1) dr = - \frac{k_F^2}{10\pi} . \quad (252)$$

The optical potential may now be evaluated by means of equations (246) and (247). The real part of the optical potential is simply the real part found on the basis of the independent-particle model multiplied by the correction factor

$$1 + \frac{1}{10\pi} \sigma k_F^2 . \quad (253)$$

For a cross section $\sigma = 40$ millibarns, the correction is some 20%. The imaginary part of the optical potential may be obtained by replacing the total cross section σ , which occurs in the expression for the independent-particle model, by the quantity

$$\sigma + \frac{k_F^2}{20\pi} [\sigma^2 - \left(\frac{4\pi}{k} \text{Re } f(\sigma)\right)^2] \quad (254)$$

which evidently represents an effective cross section for a nucleon in a many-particle nucleus.

The effective cross section (254) has a number of interesting properties. For incident particles of sufficiently high energy the expression $(4\pi/k) \text{Re } f(\sigma)$ may be expected to be considerably smaller in magnitude than the total cross section σ of a free nucleon. (This will be particularly true when absorptive, i.e., incoherent, processes play a large role. Experimental results to date for mesons and nucleons in the Bev range are consistent with assuming $\text{Re } f(\sigma) = 0$.) We must therefore expect that at such energies the effective cross section of a nucleon in the nucleus will

exceed the free particle cross section.¹⁸ This prediction contradicts an assumption that is widely made in the literature and so deserves further discussion.

It is well known that the exclusion principle leads to the suppression of certain scattering processes, those in which the final states are already occupied by similar particles. It has usually been assumed, therefore, that the effective cross section of a particle within the nucleus is smaller than that of a free particle. Many calculations have been performed, either with the Born approximation or the single-scattering approximation (impulse approximation), to bear this point out. It would, in fact, be a simple matter to calculate the cross section of a Fermi gas on the basis of the single-scattering approximation (207). The effective cross section per nucleon that results is an expression similar to the effective cross section implicit in (247). The expression differs, however, through the replacement of $\text{Re } f^2(\omega) = (\text{Re } f(\omega))^2 - (\text{Im } f(\omega))^2$ by $|f(\omega)|^2 = (\text{Re } f(\omega))^2 + (\text{Im } f(\omega))^2$. The latter result simply exhibits an inconsistency in the single-scattering approximation which grows in importance with the imaginary part of the forward scattering amplitude. The effects of double scattering and the interference of double and single scattering are responsible for changing the sign of the correlation term at high energies, i.e. where $(\text{Im } f(\omega))^2$ is the dominant term.

The influence of the correlation effect may be understood in a fairly simple way, geometrically. For this purpose we recall that in the absence of correlations, i.e., in the independent particle model, the effective cross section of a nucleon is just the free particle cross section. The simplest influence of correlation upon the scattering is felt through interference effects. In a Fermi gas each particle is surrounded by a hole in the distribution of similar particles. Since a uniform distribution would lead to no interference effects, the scattering by the particles absent from the hole may be seen to interfere destructively with the scattering by the nucleon at its center. This destructive interference effect is precisely what is described by the single-scattering approximation. If the correlation length ℓ greatly exceeds the wavelength, the interference correction to the cross section of a nucleon is negative and of the order of

$$\begin{aligned} \left(\frac{4\pi}{k\ell}\right)^2 |f(\omega)|^2 &= \left(\frac{4\pi}{k\ell}\right)^2 \{(\text{Re } f(\omega))^2 + (\text{Im } f(\omega))^2\} \\ &= \left(\frac{4\pi}{k\ell} \text{Re } f(\omega)\right)^2 + \frac{\sigma^2}{\ell^2}, \end{aligned} \quad (255)$$

for each of the $\sim n\ell^3$ particles correlated with it.

In extending the picture to include multiple collisions we must remember that double and triple scattering, etc., are already present in the independent-particle model. Their effects are simply accounted for by use of the free nucleon cross section in calculating the imaginary part

of the optical potential. (I. e., the phase shift function for an independent-particle nucleus is proportional to $f(\omega)$ and is given by (217). The formula for the nuclear scattering amplitude contains the exponential of this function. If the exponential is expanded in a power series, its successive terms represent the contributions of successive orders of multiple collisions.) Since the effect of multiple scattering is already accounted for implicitly when the nucleon positions are distributed randomly, we have only to account for the changes introduced by correlations. Consider a particular pair of nucleons a correlation length apart. Double scattering effects (more generally including shadowing effects as well) will change their combined total cross section by an amount of order σ^2/l^2 , i. e., by an amount precisely comparable to the contribution of $|Im f(\omega)|$ to the interference effect (255). Thus double scattering and interference effects must be considered together when the forward scattering amplitude is predominantly imaginary.

The sign of the correlation effect and a number of its properties are made clear by recalling the "eclipse" effect in the deuteron, which was discussed in an earlier section. The total cross section of a deuteron at high energies is always found to be smaller than the sum of the two free nucleon cross sections. The reason for this was shown to lie in the way shadowing and double scattering effects dominate the corrections to the cross section. The treatment of the spatial correlation of nucleons within a Fermi gas poses a problem which is in a sense the reverse of the deuteron problem. Particles which are held together by an attractive force in the deuteron are kept apart by the exclusion principle in a Fermi gas. The anticorrelation of the Fermi particles simply reverses the sign of the effect. The tendency of particles to remain apart from one another in a Fermi gas means that they tend to remain outside the regions of "shadow" cast by their neighbors. They thus present a more effective target area to the incident beam than if their relative positions were random. It is for this reason that the effective cross section of a nucleon exceeds the free particle cross section at high energies.

Although the correction added to the free particle cross section is positive at high energies, it should be emphasized that the correction goes over into the more familiar negative one as the energy decreases. As the incident energy descends the imaginary part of the forward scattering amplitude, $|Im f(\omega)| = k\sigma/4\pi$, decreases in magnitude until it is dominated by $|Re f(\omega)|$. In that limit the long-standing estimates based upon the single-scattering approximation become more nearly correct.

We have thus far assumed that the incident particle is not a nucleon in order to confine the application of the exclusion principle to the nuclear wave function. If the incident particle is a nucleon the entire system, nucleus plus incident particle, must be described by an anti-symmetric wave function. Exchange processes then become possible; i. e., the nucleon which leaves the nucleus is different from the one that enters. Such processes are indistinguishable from other forms of elastic scattering and interfere coherently with them. Although exchange pro-

cesses may contribute significantly to the scattering at low energies, we shall show that they are of little importance in the high-energy limit.

Consider the scattering of a pair of (non-identical) nucleons in their center of mass system. Suppose that the scattering amplitude for one of them is $f(\vartheta)$. If the nucleons are now considered to be identical particles, antisymmetrization of the wave function yields the scattering amplitudes $f(\vartheta) \pm f(\pi-\vartheta)$ for the singlet and triplet states. The domain of the angular argument ϑ , for these amplitudes, must be restricted to a single hemisphere, say, $0 \leq \vartheta \leq \frac{\pi}{2}$. The superposition expresses our inability to say whether, speaking in classical terms, a scattering through the angle ϑ or $\pi-\vartheta$ actually takes place. For angles ϑ at which the amplitudes $f(\vartheta)$ and $f(\pi-\vartheta)$ are both large, their interference may be important. In the high-energy limit, however, the scattering is characterized by extreme anisotropy; $f(\vartheta)$ is very large for small ϑ and quite small for all other directions. The only angles in the range $0 \leq \vartheta \leq \pi/2$ for which $|f(\vartheta)| \pm |f(\pi-\vartheta)|$ takes on large values lie close to the forward direction. For such angles the exchange amplitude $f(\pi-\vartheta)$ is negligibly small; i.e., it is very much more probable that the scattering takes place through the small angle ϑ than through the angle $\pi-\vartheta \approx \pi$. The assumption that back-scattering is extremely weak, in fact, underlies most of our approximation methods.

Since the exchange amplitude is negligible, it is clear that the same result would have been obtained by foregoing the procedure of antisymmetrization altogether. This result may be stated a bit differently by noting that the strong anisotropy of the scattering means that large values of the orbital angular momentum are contained in the scattered wave. The effect of the exclusion principle disappears since we are at the limit in which the angular momenta may be treated semiclassically.

The exchange effects, which are negligible in the center of mass frame of two nucleons, are equally negligible in the laboratory system. They may with similar accuracy be neglected in treating collisions of the incident nucleon with a succession of nucleons within a nucleus. We conclude, therefore, that the results derived in this and earlier sections should hold to fair accuracy when the incident particles are nucleons, as well as any other types of particles.

The Optical Model for Nuclei of Arbitrary Radius

The expressions for the optical potential in the preceding sections have been evaluated under the assumption that the nuclear radius and correlation length are much greater than the range of interaction of a nucleon with the incident particle. Although this assumption has been convenient in simplifying the derivations, it is clearly not too accurately fulfilled in practice. By using it we have gained a certain geometrical insight into the optical model as well as the generalization of a number of results which have been widely discussed in connection with theories of (infinite) nuclear matter. In the present section we shall indicate briefly how the calculations may be generalized to treat nuclei of arbitrary dimensions.

The assumptions which restrict the radii were made as a means of simplifying certain integrations over the configuration space of the nucleons. In particular, it was assumed that the functions $\Gamma_j(b) = 1 - e^{i\chi_j(b)}$ are of such short range, compared to nuclear dimensions, that the variations of nuclear density functions, etc., within this range are negligible. All of the information required about the scattering by the individual nucleons was therefore contained in the integral

$$\int \Gamma_j(b) d^{(2)}b = (2\pi/i\kappa) f_j(0).$$

In order to deal with nuclei of smaller radius, or with longer range interactions, more detailed knowledge of the functions $\Gamma_j(b)$ is clearly necessary. The values of these functions, however, are not, in general, directly available from experiment. The procedure by which they are to be found is essentially that of phase shift analysis. Within the scope of the present approximations this analysis is conveniently simple. The function $\Gamma_j(b)$ may be directly expressed as a fourier transform of the scattering amplitude. For this purpose we shall write the scattering amplitude $f(k', \bar{k})$ hereafter simply as a function of the momentum transfer $\bar{k} - \bar{k}'$; i.e., we shall write $f(\bar{k} - \bar{k}')$ in place of $f(\bar{k}', \bar{k})$, omitting explicit reference to the energy parameter κ , which remains constant throughout. With this notation the scattering amplitude is given in terms of $\Gamma_j(\bar{b})$ by the integral (203),

$$f_j(\bar{k} - \bar{k}') = \frac{i\kappa}{2\pi} \int e^{i(\bar{k} - \bar{k}') \cdot \bar{b}} \Gamma_j(\bar{b}) d^{(2)}b. \quad (256)$$

The function Γ_j may be solved for in terms of f_j by means of a two-dimensional fourier transformation,

$$\Gamma_j(\bar{b}) = \frac{1}{2\pi i\kappa} \int e^{-i\bar{\lambda} \cdot \bar{b}} f_j(\lambda) d^{(2)}\lambda. \quad (257)$$

The vector variable of integration $\bar{\lambda}$ in this integral is conjugate to the impact vector \bar{b} . It is taken to vary over the plane perpendicular to the incident propagation direction \bar{k} .

Some practical limitations inherent in the above solution for Γ_j should be borne in mind. The scattering amplitude f_j upon which it is based is, in general, a complex function of the momentum transfer. The usual experiments, measuring scattered intensities, tell us only the modulus of this function (for non-vanishing momentum transfer). Knowledge of the phase of the scattering amplitude must therefore be procured from other sources. (E.g., if the interaction is purely absorptive f_j is pure imaginary.) Furthermore at any given energy only a finite range of momentum transfers, i.e., $0 \leq \lambda \leq 2\kappa$, is physically available. Never-

theless the integration (257) extends over an infinite range of momentum transfers. The impossibility of measurement in the region $\lambda \geq 2k$ leads, in fact, to very little uncertainty under conditions suited to the high-energy approximation; i.e., the scattering amplitude is highly peaked in the forward direction and may, to the present accuracy, be considered to vanish for such large momentum transfers.

To evaluate the optical phase shift function for arbitrary radii we need only substitute the expression (257) for $f(\vec{\lambda})$ into the general expressions (210) or (214) for $X_{\text{opt}}(\vec{b})$. In this way we find

$$X_{\text{opt}}(\vec{b}) = \frac{N}{2\pi k} \int e^{-i\vec{\lambda} \cdot (\vec{b} - \vec{s})} f(\vec{\lambda}) \rho(\vec{q}) d^{(2)}\lambda d\vec{q}. \quad (258)$$

On introducing the form factor for the density ρ ,

$$S(\lambda) = \int e^{i\vec{\lambda} \cdot \vec{r}} \rho(r) d\vec{r}, \quad (259)$$

the optical phase shift may be written as

$$X_{\text{opt.}}(\vec{b}) = \frac{N}{2\pi k} \int e^{-i\vec{\lambda} \cdot \vec{b}} f(\lambda) S(\lambda) d^{(2)}\lambda \quad (260)$$

$$= \frac{N}{k} \int_0^\infty J_0(\lambda b) f(\lambda) S(\lambda) d^{(2)}\lambda. \quad (261)$$

Since the functions f and S depend only on $|\vec{\lambda}|$, it is a simple matter to construct a spherically symmetric potential which leads to the phase shift function (260). Let us consider the optical potential given by the three-dimensional Fourier integral

$$-\frac{1}{\hbar r} V_{\text{opt.}}(r) = \frac{N}{(2\pi)^3 k} \int e^{-i\vec{\lambda} \cdot \vec{r}} f(\lambda) S(\lambda) d^{(3)}\lambda \quad (262)$$

$$= \frac{N}{\pi k} \int_0^\infty \frac{\sin \lambda r}{r} f(\lambda) S(\lambda) \lambda d\lambda. \quad (263)$$

This potential is clearly spherically symmetric. Furthermore integration along the z -axis shows directly its correspondence to the phase shift (260). As an alternative derivation of this expression we may substitute the phase shift function (261) in the explicit formula (201) for the solution of the Abel integral equation which defines the potential. The latter procedure shows the uniqueness of the solution. Contact may be made with our earlier work by noting the behavior of (262) as the nuclear radius be-

comes large compared with the interaction radius. In that limit the function S becomes so strongly peaked in the forward direction that the scattering amplitude $f(\lambda)$ in the integrand may be replaced by $f(0)$. The expression then reduces to (218). The expression (263) is of just the form one would find by treating single scattering only, and using the Born approximation for V_{opt} . Once again we must emphasize that the present treatment accounts fully for multiple scattering, and assumes the particles uncorrelated.

The construction of the optical phase shift function is equally simple in the presence of spin-orbit forces. For this purpose we need only substitute the expression (133) for the spin-dependent scattering amplitude in (260). We then find

$$\chi_{\text{opt}}(b) = \frac{N}{2\pi k} \int e^{i\vec{\lambda} \cdot \vec{b}} \left\{ f(\lambda) + \vec{\sigma} \cdot \left(\frac{\vec{\lambda} \times \vec{k}}{\lambda k} \right) g(\lambda) \right\} S(\lambda) d^{(2)}\lambda. \quad (264)$$

This phase shift function corresponds to the spin-orbit potential

$$-\frac{1}{k r} V_{\text{opt}}(r) = \frac{N}{(2\pi)^2 k} \int e^{i\vec{\lambda} \cdot \vec{r}} \left\{ f(\lambda) + \vec{\sigma} \cdot \left(\frac{\vec{\lambda} \times \vec{k}}{\lambda k} \right) g(\lambda) \right\} S(\lambda) d^{(3)}\lambda. \quad (265)$$

Another point at which the nucleon interaction range was assumed relatively small occurred in the discussion of correlation effects. There it was assumed that the correlation length as well as the nuclear radius considerably exceeds the interaction range. Since nuclear forces will tend to produce correlations within distances of the order of their own ranges, it is most important that this restriction on the correlation length be relaxed. The calculation of the optical phase shift function may again be carried out by substitution of (257) in a general expression derived earlier, this time Eq. (240). We shall quote the result for the case in which the nuclear radius remains large compared to both the correlation length l and the interaction radius a , but the latter lengths may be arbitrarily related to one another. The change of the optical phase shift function due to pair correlations is then

$$\delta[\chi_{\text{opt}}(b)]_{\text{corr.}} = \frac{i}{2k^2} \int e^{i\vec{\lambda} \cdot \vec{s}} [g(q) - 1] f^2(\lambda) d^{(2)}\lambda d\vec{q}. \quad (266)$$

$$\int_{-\infty}^{\infty} n^2(b, z) dz.$$

^{*} If we define the form factor, $C(\lambda)$, of the correlation function as

$$C(\lambda) = \int e^{i\vec{\lambda} \cdot \vec{r}} [g(r) - 1] d\vec{r},$$

the phase shift correction reduces to

$$\delta[X_{\text{opt}}(b)]_{\text{corr.}} = \frac{i}{2k^2} \int f^2(\lambda) C(\lambda) d^{(1)}\lambda \cdot \int_{-\infty}^{\infty} n^2(b, z) dz. \quad (267)$$

Since the density function $n(b, z)$ is spherically symmetric, the correlation correction to the optical potential is given by

$$-\frac{1}{\hbar v} \delta[V_{\text{opt}}(r)]_{\text{corr.}} = \frac{i}{2k^2} n^2(r) \int f^2(\lambda) C(\lambda) d^{(1)}\lambda. \quad (268)$$

In the limit of large correlation lengths this expression reduces to (245).

Our discussion of the correlations brought about by the exclusion principle may now be extended by finding the fourier transform, $C(\lambda)$, of the correlation function (250). This calculation corresponds simply to finding the common volume in momentum space of two Fermi spheres whose centers are displaced by a distance λ relative to one another. Its result is

$$C(\lambda) = \begin{cases} -\frac{9m^2}{k_F^3} \left\{ \frac{2}{3} - \frac{1}{2} \frac{\lambda}{k_F} + \frac{1}{24} \frac{\lambda^3}{k_F^3} \right\} & \text{for } 0 \leq \lambda \leq 2k_F \\ 0 & \text{for } 2k_F \leq \lambda. \end{cases} \quad (269)$$

Hence the effect of the exclusion principle on the optical potential is given by the simple integral

$$\begin{aligned} -\frac{1}{\hbar v} \delta[V_{\text{opt}}(r)]_{\substack{\text{excl.} \\ \text{princ.}}} &= \\ -\frac{i}{4\pi k^2} \int_0^{2k_F} f^2(\lambda) \left\{ \frac{2}{3} k_F^3 - \frac{1}{2} k_F^2 \lambda + \frac{1}{24} \lambda^3 \right\} \lambda d\lambda. \end{aligned} \quad (270)$$

In the preceding section we noted the close correspondence between the correlation effect in nuclei and the "eclipse" effect in the deuteron. In the discussion of the eclipse effect the calculations were also

simplified at one point by the assumption that the interaction range is much smaller than the deuteron radius. This assumption may likewise be removed by making use of the expression (257) for $\bar{\gamma}$. The generalization of the expression (184) for the deuteron total cross section, which we reach in this way, is

$$\sigma_d = \sigma_n + \sigma_p + \frac{2}{k^2} \int S(\lambda) \operatorname{Re}\{f_n(\lambda)f_p(\lambda)\} d^{(2)}\lambda, \quad (271)$$

where $S(\lambda)$ is the deuteron form factor

$$S(\lambda) = \int e^{i\vec{\lambda} \cdot \vec{r}} |u(r)|^2 d\vec{r}. \quad (272)$$

The expression (271) reduces to (184) in the limit of large deuteron radii. It should be a considerably more accurate expression to use in analyzing experimental data, but its use requires some knowledge of the angular distributions of scattering.

Inelastic Scattering

The optical model, as we have discussed it thus far, represents an approach to the problem of elastic scattering. In the present section we shall indicate briefly how it may be employed in treating inelastic transitions as well as elastic ones. We shall then devote a few remarks to some of the more general properties of inelastic scattering at high energies.

We have already derived a general expression for the inelastic scattering amplitude of an incident particle by a many-particle system, e.g., a nucleus. As long as the energy difference between the initial nuclear state, i , and the final state, f , is small compared to the incident energy, the scattering amplitude is given by (172),

$$F_{fi}(\vec{k}', \vec{k}) = \frac{k}{2\pi i} \int e^{i(\vec{k}-\vec{k}') \cdot \vec{b}} d^{(2)}b \cdot \\ \int u_f^*(\vec{q}_1, \dots, \vec{q}_N) \left\{ e^{i \sum_j X_j (\vec{b} - \vec{s}_j) - 1} \right\} u_i(\vec{q}_1, \dots, \vec{q}_N) \prod_j d\vec{q}_j. \quad (172)$$

Since the nucleus changes its state in the course of a collision for $f \neq i$, quantities which enter the integrand of (172) can no longer be described entirely in terms of static density and correlation functions. In practice a model of some sort must always be used to provide suitable initial and final state wave functions. Many such models have been devised and we shall not enter into their details here, other than to mention a simplifying feature which most of them share. It appears that many transitions may

be described as involving a change of state of only a very small number of nucleons. The remaining nucleons, e.g., those in closed shells, play no active role in the transition. It is not difficult to show that the treatment of such transitions may be carried out by explicitly describing the collision of the incident particle with the small group of nucleons, and allowing the collision to take place within an optical potential well which is produced by the remaining (inert) nucleons.

The simplest such model is one in which a single nuclear particle is assumed to make a transition. We separate its wave function from that of the remaining nucleons by writing

$$\psi_i(\vec{q}_1, \dots, \vec{q}_N) = \nu_i(\vec{q}_1) \psi(\vec{q}_2, \dots, \vec{q}_N) , \quad (271)$$

$$\psi_f(\vec{q}_1, \dots, \vec{q}_N) = \nu_f(\vec{q}_1) \psi(\vec{q}_2, \dots, \vec{q}_N) .$$

An optical phase shift function

$$\chi_{\text{opt}}^{(N-1)}(\vec{b})$$

may then be defined for the system of $N-1$ inert particles by means of the relation

$$e^{i\chi_{\text{opt}}^{(N-1)}(\vec{b})} = \int |\psi(\vec{q}_2, \dots, \vec{q}_N)|^2 e^{i \sum_{j=2}^N \chi_j(\vec{b} - \vec{s}_j)} \pi d\vec{q}_j . \quad (272)$$

With this definition, the scattering amplitude (172) may be written as

$$\begin{aligned} F_i(\vec{k}', \vec{k}) &= \frac{k}{2\pi i} \int e^{i(\vec{k} - \vec{k}') \cdot \vec{b}} d^{(2)} b \cdot \\ &\quad \int \nu_f^*(\vec{q}_1) \left\{ e^{i\chi_{\text{opt}}^{(N-1)}(\vec{b}) + i\chi_1(\vec{b} - \vec{s}_1) - 1} \right\} \nu_i(\vec{q}_1) d\vec{q}_1 \\ &= \int \nu_f^*(\vec{q}_1) e^{i(\vec{k} - \vec{k}') \cdot \vec{s}_1} \nu_i(\vec{q}_1) \cdot \\ &\quad \frac{k}{2\pi i} \int e^{i(\vec{k} - \vec{k}') \cdot (\vec{b} - \vec{s}_1)} \left\{ e^{i\chi_{\text{opt}}^{(N-1)}(\vec{b}) + i\chi_1(\vec{b} - \vec{s}_1) - 1} \right\} d^{(2)} b d\vec{q}_1 . \end{aligned} \quad (273)$$

This expression falls into the general form

$$F_{fi}(\vec{k}', \vec{k}) = \int v_f(\vec{q}_i) e^{i(\vec{k}-\vec{k}') \cdot \vec{s}} \bar{f}(\vec{k}', \vec{k}, \vec{s}) v_i(\vec{q}_i) d\vec{q}_i , \quad (274)$$

where $\bar{f}(\vec{k}', \vec{k}, \vec{s})$ represents the scattering amplitude of the first nucleon, regarded not as an isolated particle, but as lying at an impact coordinate \vec{s} within a region containing an optical potential determined by the remaining $N - 1$ nucleons. These considerations are easily generalized to treat transitions of small groups of particles. Transitions of a more highly organized character, however, such as those between rotational states, require somewhat simpler models. To treat such processes the nucleus might be regarded as a rigid or fluid continuum, and the corresponding phase shift functions employed.

Since energy discrimination poses a difficult experimental problem in dealing with highly energetic particles, it probably will not be practical to observe individually very many examples of particular inelastic transitions. It will be much easier, instead, to observe angular distributions of the total inelastic scattering. In the high-energy limit, as we have noted, forward scattering will be intense and the energy transfers in inelastic scattering will be predominantly quite small. The scattered intensities may then be summed over all final states to good approximation by using the completeness relation (164). To find the angular distribution of inelastic or incoherent scattering, we subtract from this sum the elastic scattering intensity. The resulting inelastic differential cross section may be written as

$$\sum_{f \neq i} |F_{fi}(\vec{k}', \vec{k})|^2 = \left(\frac{k}{2\pi} \right)^2 / e^{i(\vec{k}-\vec{k}') \cdot (\vec{b}-\vec{b}')} \left\{ \left\langle e^{i \sum_j X_j (\vec{b}-\vec{s}_j)} e^{-i \sum_i X_i^* (\vec{b}'-\vec{s}_i)} \right\rangle_i - \left\langle e^{i \sum_j X_j (\vec{b}-\vec{s}_j)} \right\rangle_i \left\langle e^{-i \sum_i X_i^* (\vec{b}'-\vec{s}_i)} \right\rangle_i \right\} d^{(n)} b d^{(n)} b' \quad (275)$$

$$= \left(\frac{k}{2\pi} \right)^2 / e^{i(\vec{k}-\vec{k}') \cdot (\vec{b}-\vec{b}')} \left\{ \left\langle \prod_j (1 - \Gamma_j(\vec{b}-\vec{s}_j)) \times [1 - \Gamma_j^*(\vec{b}'-\vec{s}_j)] \right\rangle_i - \left\langle \prod_j (1 - \Gamma_j(\vec{b}-\vec{s}_j)) \right\rangle_i \left\langle \prod_i (1 - \Gamma_i^*(\vec{b}'-\vec{s}_i)) \right\rangle_i \right\} d^{(n)} b d^{(n)} b' , \quad (276)$$

where the brackets $\langle \rangle_i$ again signify the expectation value in the initial nuclear state. The expression (276) contains the expectation values of products rather similar in form to those which occurred in the discussion of the optical model. We shall omit the details of their evaluation here and simply quote the form to which the inelastic angular distribution may be reduced, when certain assumptions we have discussed earlier are introduced. If we assume that the interaction range of a nucleon is much smaller than the nuclear radius, and that the nucleons are independent particles, we find

$$\begin{aligned} \left(\frac{d\sigma}{d\Omega} \right)_{\text{inelast.}} &= \sum_{f \neq i} |F_{fi}(\vec{k}, \vec{k}')|^2 \\ &= \left(\frac{k}{2\pi} \right)^2 \int d^{(2)}B e^{-\sigma \int_{-\infty}^{\infty} n(\vec{B}, z) dz} \int d^{(2)}\beta e^{i(\vec{k}-\vec{k}') \cdot \vec{\beta}} \cdot \\ &\quad \left\{ e^{\frac{1}{k^2} / e^{-i\vec{\lambda} \cdot \vec{\beta}} |f(\lambda)|^2 d\lambda} \int_{-\infty}^{\infty} n(\vec{B}, z) dz - 1 \right\}, \end{aligned} \quad (277)$$

where the vector variables of integration are related to the variables of (276) by

$$\vec{B} = \frac{1}{2}(\vec{b} + \vec{b}') , \quad \vec{\beta} = \vec{b} - \vec{b}' . \quad (278)$$

Some insight into the nature of the expression (277) for the inelastic differential cross section may be obtained by expanding its integrand in powers of the nucleon cross section. To lowest order we find

$$\begin{aligned} \left(\frac{d\sigma}{d\Omega} \right)_{\text{inelast.}} &= \frac{1}{(2\pi)^2} \int d^{(2)}B \int d^{(2)}\beta e^{i(\vec{k}-\vec{k}') \cdot \vec{\beta}} \int e^{i\vec{\lambda} \cdot \vec{\beta}} |f(\lambda)|^2 d^{(2)}\lambda \cdot \\ &\quad \int_{-\infty}^{\infty} n(\vec{B}, z) dz + \dots \\ &= N |f(k-k')|^2 + \dots , \end{aligned} \quad (279)$$

which is just the sum of the intensities of single scattering by the individual nucleons. The higher order terms correct for multiple collisions, which are important when the nucleus has appreciable opacity.

Another expression which illustrates the meaning of (277) is the total inelastic cross section. The angular distribution (277) may be integrated over directions of \vec{k}' by means of the approximation (94). The result is

$$\sigma_{\text{inelast.}} = \int d^{(2)}B e^{-\sigma \int_{-\infty}^{\infty} n(\vec{B}, z) dz} \left\{ e^{-\int |f(\lambda)|^2 d^{(2)}\lambda / k^2} \int_{-\infty}^{\infty} n(\vec{B}, z) dz - 1 \right\} , \quad (280)$$

Under the approximation (94) the integral

$$\frac{1}{k^2} \int |f(\lambda)|^2 d^{(2)}\lambda$$

is simply the total scattering cross section of a nucleon, $\sigma_{\text{scatt.}}$. If processes other than simple nucleon-nucleon scattering are present, their effect upon the scattering is described in terms of an absorption; i.e., we write $\sigma = \sigma_{\text{abs.}} + \sigma_{\text{scatt.}}$. Thus the inelastic cross section may be written as

$$\sigma_{\text{inelast.}} = \int d^{(2)}B e^{-\sigma_{\text{abs.}} \int_{-\infty}^{\infty} n(\vec{B}, z) dz} \left\{ 1 - e^{-\sigma_{\text{scatt.}} \int_{-\infty}^{\infty} n(\vec{B}, z) dz} \right\}. \quad (281)$$

This expression has a simple interpretation. It shows that the inelastic cross section is just the integral over impact parameters of the probability that the incident particle both escapes absorption and undergoes at least one scattering collision.

It is also possible to calculate the effect of nucleon position correlations on the angular distribution of inelastic scattering. In particular, the correlations due to the exclusion principle are of some interest in their effect on the inelastic scattering near the forward direction. This calculation is a simple application of the methods we have discussed, but would be a bit lengthy to present here.

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