BRUECKNER THEORY OF NUCLEI

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BRUECKNER THEORY OF NUCLEI*

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Abstract:

This paper reviews developments of the Brueckner theory of nuclei, starting with the multiple-scattering approach in the 1954 papers of Brueckner et al. Inevitably, the presentation represents the authors personal view on the problems. Theories rather than calculations have been emphasized. The latter depend very much upon the two-nucleon interaction which is still not known in sufficient detail. The definition of the Brueckner reaction-matrix is discussed at some length with regard to insertions in hole- and particle-lines. Löwdin's Exact Self-Consistent-Field theory that provides an exact many-body reaction matrix is given a short presentation for comparison with Brueckner's theory as applied to finite nuclei. Considerable attention has been given to the shell-model potential required for calculations on finite nuclei. The concept of single-particle energies is discussed in some detail in relation to removal energies. Some numerical results are reviewed either for illustrating the theory or because they are recent.

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1. Introduction

One of the primary aims of a microscopic theory of nuclei is to describe the saturation and binding of nuclear matter. These features are related to the nature of nuclear forces and to many-body effects. Early efforts to explain the saturation effect went by way of monotonic forces with exchange effects [1]. The amount of exchange that was found necessary for saturation did however not agree with the knowledge of nuclear forces obtained from free scattering experiments. An explanation purely in terms of many-body forces [2] did not seem satisfactory either [3]. The energy dependence of the S-wave phase shift led Jastrow [4] to suggest a force that is strongly repulsive at short distances. The study of a many-body problem with strong forces was however not possible by Born or Hartree–Fock methods which were the conventional methods prior to 1954. In the pioneering work by Brueckner, Levinson and Mahmoud [3] the methods developed by Watson [5] to treat the problem of multiple scattering were revised for solving the ground state problem of nuclei.

Brueckner later changed his approach by using perturbation-theoretical methods [6]. These have become very powerful for the treatment of many-body systems by the establishment of the linked cluster expansion. The general proof of this was first given by Goldstone [7], who applied methods developed in field theory. The field theoretical use of diagrams introduced by Feynman has also proven useful for the nuclear many-body problem. Extensive discussions of these diagrammatic methods applied to many-body problems have been made by other authors [8–10], and can also be found in textbooks [11, 12]. Much of our presentation here is based upon these methods but we shall only discuss some aspects relevant to our discussions.

The elegance of the Brueckner theory stems largely from the replacement of the strong v-interaction by a much smoother K-interaction; in the literature also referred to as G or t. This interaction corresponds to a partial summation of diagrams. The beauty of the theory is that, according to the present understanding, the important diagrams are summed by the relatively simple operator K, which formally represents a two-body interaction allowing for many-body effects.

In this article the aim has been to present a short but comprehensive report on the developments of the Brueckner theory from the first paper in 1954 till the latest works.

Numerical results are not discussed in much detail other than for illustrating the theory. Some recent results are also reviewed but the reader is in this regard referred to the review article by Bethe [13].

During the 60's much of the nuclear many-body work centered around the problem of calculating the K-matrix. Some of the methods used to calculate the K-matrix in nuclear matter have been discussed by Sprung [14].

2. The Hartree–Fock method

The Hartree–Fock method has been of great importance for solving the many-electron problem of atoms. Because the nuclear forces are so much stronger, this method is not equally well applicable to nuclei. However, it is relatively simple and well understood and therefore provides a natural introduction to the more complex nuclear problem. It also contains some features that we shall make direct use of subsequently.

The Hamiltonian of a many-body system of A particles, interacting via two-body forces $v(ij)$ is

$$H = \sum_{i=1}^{A} T(i) + \tfrac{1}{2} \sum_{i \neq j}^{A} v(ij) \tag{2.1}$$

where $T(i)$ denotes kinetic energies.

Choosing any Hamiltonian H_0 such that

$$H_0 = \sum_{i=1}^{A} (T(i) + V(i)) \tag{2.2}$$

where $V(i)$ are one-body potentials, one can write

$$H = H_0 + H' \tag{2.3}$$

where

$$H' = \tfrac{1}{2} \sum_{ij} v(ij) - \sum_{i} V(i) \,. \tag{2.4}$$

Assuming the eigenstates of H_0 to be known one can make a perturbation expansion in terms of H'. This expansion is conveniently made following the rules of the linked cluster theorem and visualized by the Goldstone diagrams [7]. We shall make more extensive use of these methods in sect. 3 where a short description of diagrammatic notations is found.

The few lowest order energy-diagrams are shown in fig. 1. Assuming that this series converges, it is in principle possible to calculate the energy to any degree of accuracy by successively calculating the terms of the series represented by the diagrams. Although the formal expansion is valid for any choice of H_0 one will find that the rate of convergence will depend, among other things, on the choice of H_0, that is on the choice of V. By defining the particle–hole matrix elements of V to be equal to the sum of all v-interactions (including exchange) one is able to cancel particle–hole excitations. All diagrams 1b will for example cancel against each other by this definition.

The Hartree–Fock choice of the potential V is

$$V_{\mathrm{HF}} = \sum_{j} (\phi_j | v \phi_j) + \text{exchange} \tag{2.5}$$

where ϕ_j are the single-particle wavefunctions determined by the Hamiltonian (2.2), with $V = V_{\mathrm{HF}}$. After iteration until self-consistency one achieves that all diagrams with v-insertions not only at

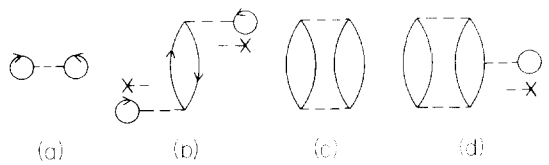

Fig. 1. Goldstone diagrams corresponding to the perturbation H' in eq. (2.4). The crosses represent V-interactions.

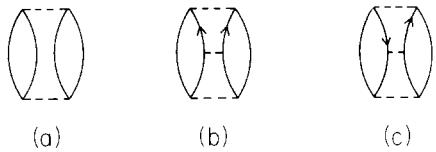

Fig. 2. Correlation energy diagrams calculated by Kelly [16].

vertices but also in lines will cancel against a V-interaction. This cancellation is of great practical importance because it would be quite complicated to calculate all these diagrams and they are physically very important. It may not be of much importance that diagram 1d is cancelled, because the similar but lower order diagram shown in fig. 1c is not cancelled by the Hartree–Fock approximation. This latter diagram contributes to the correlation energy. This energy, E_{corr} is in atomic physics often *defined* by

$$E_{\text{corr}} = E_{\text{nr}} - E_{\text{HF}} \tag{2.6}$$

where E_{nr} is the ground state energy of the nonrelativistic Hamiltonian [15].

Correlation energies have been calculated for atoms by Kelly [16], using diagrammatic methods. Some of the diagrams considered by Kelly are shown in fig. 2. He uses a two-stage procedure by first finding the Hartree–Fock field and then calculating the correlation diagrams in that basis set. This method can in principle be used for any many-body problem. The magnitude of the correlations depends of course very much on the two-body interaction and also on the density. For the electron system it has however been demonstrated to depend also on the geometry of the system. Gell-Mann and Brueckner showed that ring-diagrams are important for an electron-gas [17]. These diagrams are responsible for the screening and the collective plasma-oscillations. They are however not important for the finite system. It was shown explicitly by Ma and Brueckner that this can be ascribed to the large density gradients in the atom [18]. It can also be interpreted as the effect of the strong central Coulomb-field on the perturbation expansion for atoms.

A major difference between the electron system and the nuclear system is the strength of the two-body force. Another difference is of course that for atoms there is the strong Coulomb field due to the nuclear proton charge, while in nuclei the field is generated totally by the nucleons themselves. We saw above that the nuclear Coulomb-field has a stabilizing effect on the atomic electron system. The nuclear field on the other hand is totally determined by the self-consistency requirement. This may in itself explain why collective phenomena are more important for nuclei than they are for atoms.

The Coulomb force is well known while our knowledge of the nucleon–nucleon force still is incomplete, especially what concerns the short ranged behavior ($r < 1$F). Scattering experiments can be described by either a strong short ranged repulsion, for $r \lesssim 0.5$ F, or by a momentum dependence (non-locality) such that the force becomes increasingly repulsive with increasing energy. Theoretical investigations seem to favor the latter type of interaction, although they have as yet not been used as extensively as conventional local (local in the radial coordinate that is) forces.

Correlations can in principle (disregarding the singular, hard-core interaction suggested by Jastrow [4]) be calculated for nuclei just as they are calculated for atoms. The practical complication is that they become quite large and often are very tedious and complicated to calculate with

the nucleon force as we know it today. There does however exist appreciable uncertainty in the determination of the nucleon potential from low energy scattering data alone, and the binding of a nucleus is in some sense a low energy problem. It is possible to construct smooth potentials that agree well with low energy scattering data and such potentials will give relatively small two-body correlations. This approach has been taken by Kerman, Bassichis et al. [19, 20] and by Riihimaki [12, 21]. The difficulty encountered in this approach is that the correlation terms are still fairly large especially because of the tensor force. It is in the author's opinion somewhat disconcerting to have a procedure which adjusts the interaction in order to simplify the calculation, and the simplifications appear furthermore somewhat dubious. It seems a great deal more satisfying to start with an interaction that incorporates as much as possible of the experimental and theoretical knowledge that we do have of the two-nucleon force. This knowledge seems to favor a soft repulsive core (maybe also a nonlocality in the radial dependence) over a hard core. The interaction is nevertheless so strong and has such a strong tensor component, that the correlation terms become quite large. The two-stage approach is therefore not as practical for nuclei as it is for atoms.

3. The Brueckner method; the reaction-matrix

A technique to overcome the problem of the large two-body correlations was initiated by Brueckner and coworkers. The technique was originally applied to a hard-core interaction, which was an accepted nucleon–nucleon potential at the time that the technique was first developed [3, 4, 6, 22]. The initial work was inspired by the multiple scattering theory of Watson [5], which is described briefly below.

The development of Watson's theory of the multiple scattering of a particle by a quantum mechanical many-body system was influenced by the multiple scattering theory of light developed by Lax and Foldy [23]. The theory stresses the distinction between coherent and incoherent scattering. In incoherent scattering the many-body system is excited and the outgoing wave resulting from this excitation does not interfere with the elastically scattered wave. This distinction is formally made by separating the scattering matrix t_α for a pair of particles in the medium, into a coherent and an incoherent part. Thus

$$t_\alpha = t_{C\alpha} + I_\alpha \tag{3.1}$$

where

$$t_\alpha = v_\alpha + v_\alpha \frac{1}{E - H_0 - V_C \pm i\epsilon} t_\alpha \,. \tag{3.2}$$

Here v_α is the potential between a pair of particles. It is assumed to be the same as in free scattering. Outgoing or ingoing waves are selected by choosing $+i\epsilon$ or $-i\epsilon$ respectively. V_C is the coherent potential defined by

$$V_C = \sum_\alpha t_{C\alpha} \,. \tag{3.3}$$

Here the $t_{C\alpha}$ are defined as the parts of the t_α in eq. (3.2) that are diagonal with respect to the

basis set defined by

$$(H_0+V_C)\,\psi_C = E\psi_C \tag{3.4}$$

where H_0 is the kinetic energy operator.

The exact wavefunction ψ for the many-body system is related to the approximate solution ψ_C in eq. (3.4) which was obtained by considering only coherent scatterings. The relation is

$$\psi = F\psi_C \tag{3.5}$$

where F is the solution of an integral equation containing the incoherent scatterings I that were neglected when V_C and ψ_C were defined,

$$F = 1 + \frac{1}{E-H_0-V_C} \sum_\alpha I_\alpha F_\alpha \,. \tag{3.6}$$

The formalism of Watson is very powerful in that it provides an exact solution of the problem (except for an $1/A$ approximation). Successive approximations can be made to reduce the formalism to forms that are suitable for calculation and to get a physical insight into the problem. An important reduction of the equations leads to the optical model approximation

$$V_C = \sum_\alpha t'_{C\alpha} \tag{3.7}$$

where t' are the free space scattering amplitudes obtained by neglecting V_C in eq. (3.2). This is a useful approximation because t' is readily obtainable from experimental data. It has been used by several authors, the earliest work being those by Riesenfeld and Watson [24], by Bethe [25] and by Kerman, McManus and Thaler [26]. (See also the article by Fetter and Watson [27].)

There are especially two features of the Watson theory which apparently led Brueckner and coworkers to attempt a similar approach to the ground state problem of nuclei. One is Watson's derivation of the optical model. It has always been felt that the success of the nuclear shell-model physically must be related to that of the optical model. It therefore lay near at hand to assume that a nuclear shell-model could be derived in a way similar to the derivation of the optical model. The other feature is that the optical model is constructed from scattering amplitudes as in eqs. (3.3), (3.7) and *not* from the two-body potential. The latter is finite even if the former contains singularities like a hard core.

Brueckner's initial work followed Watson's multiple scattering theory rather closely. An essential difference between the scattering and bound state problems is in the boundary conditions. This led Brueckner to modify Watson's equations by replacing the $\pm i\epsilon$ in the Green's functions by the principal value in eq. (3.2). The formal justification for this replacement was shown by Reifman, DeWitt and Newton [28]. Brueckner's scattering amplitude in the nuclear medium is therefore the same as the K-operator considered earlier by Lippman and Schwinger [29].

The first of the series of papers by Brueckner and coworkers on this subject contains an approximation referred to as the phase-shift approximation [3, 30]. In this approximation one replaces the effective interaction t_α by the free scattering amplitude t'_α in the forward direction. It is well known that this scattering amplitude is directly related to the phase-shift and it is there-

fore very simple to do a calculation in this approximation. The use of the free scattering amplitude implies neglecting V_C in eq. (3.2).

In a subsequent paper Brueckner investigated the modification of the interaction t_α by the potential V_C in eq. (3.2). This *dispersion* effect leads to a self-consistency problem because V_C does in turn depend on t_α in eq. (3.3). Brueckner discusses this problem in much detail and calculations were made [31]. It is interesting to note that following a suggestion by Wheeler, Brueckner used the effective mass approximation in this investigation by putting

$$V_C(k) = V_C(0) + bk^2 \ . \tag{3.8}$$

He therefore arrives at equations later used by Bethe, Brandow and Petschek in their reference spectrum method [32]. He also considers corrections to the effective mass approximation by the modification

$$V_C(k) = V_C(0) + bk^2 + ck^4 \ . \tag{3.9}$$

In this paper Brueckner is also aware of the correction due to the exclusion principle, although this important ingredient of the final theory was neglected at this stage of development. It is included in a later paper by Brueckner and Wada [33] (see also ref. [34]). It is interesting to observe that in this paper the idea of a local density approximation to be used for finite nuclei also was introduced and discussed in terms of a pseudo-potential. Such ideas have played an important role in the development of recent many-body theories of finite nuclei (see sect. 6.2).

Study of the higher order correction terms resulting from expansion of the F-operator in eq. (3.6) revealed the existence of *unlinked* cluster terms in the energy. Those terms are proportional to higher powers of the number of particles. Physically one expects linear terms only as the energy is an extensive function. All *linked* cluster terms do have this property. Brueckner showed that the unlinked cluster terms cancel to lowest orders. He also showed this to be the case in low order perturbation theory [35].

Goldstone proved this important linked cluster theorem for the perturbation series [7]. He applied field theoretical methods and illustrated the result by the Feynman graphs. Besides proving the linked cluster theorem the Goldstone approach and the use of diagrammatic methods have proven to provide a very convenient formulation of the Brueckner theory. It also facilitates a systematic study of higher order effects. Brandow made a further study of the algebraic methods used by Brueckner and was also able to prove the linked cluster theorem by those methods [9].

One distinguishes in Goldstone diagrams between holes (normally occupied states) and particles (unoccupied states) by representing the former by downgoing lines and the latter by upgoing lines. In what follows we shall let indices $i, j, k...$ denote holes, $a, b, c...$ denote particles and $\alpha, \beta, \gamma...$ denote either holes or particles. The propagators corresponding to these vertical lines are defined by the unperturbed Hamiltonian H_0 in eq. (2.2). Horizontal broken lines represent the V- or v-interactions of the perturbation H' in eq. (2.4). The wavy lines represent K-interactions that are defined below.

In the diagrammatic language of the Goldstone expansion, the Brueckner theory implies that some specific diagrams should be included in the approximation for the total energy. The summation of these diagrams is executed by calculating the total energy from*

* For simplicity, here and in the future, we neglect to write out the exchange terms.

$$E = \sum_i T_i + \tfrac{1}{2} \sum_{ij} K_{ij,ij} \tag{3.10}$$

where K is defined by an integral equation

$$K_{\alpha\beta,ij} = v_{\alpha\beta,ij} + \sum_{ab} v_{\alpha\beta,ab} \frac{Q}{e} K_{ab,ij}$$

$$e = e_i + e_j - e_a - e_b, \qquad e_i = T_i + V_i, \qquad e_a = T_a + V_a; \tag{3.11}$$

Q is the Pauli operator that projects out unoccupied states $a, b, \ldots$. The choice of single particle potential energies V_α determines the insertions in lines of the diagrams that are summed. In the stage of development at the time of the nuclear matter paper by Brueckner and Gammel [22] the diagrams in fig. 3 were summed by choosing

$$V_i = \sum_k K_{ik,ik} \tag{3.12}$$

while V_a was calculated from

$$V_a = \sum_k K'_{ak,ak} \tag{3.13}$$

with

$$K'_{\alpha\beta,ak} = v_{\alpha\beta,ak} + \sum_{a'b'} v_{\alpha\beta,a'b'} \frac{Q}{e'} K'_{a'b',ak} \,. \tag{3.14}$$

The energy denominator e' is here different from e in eq. (3.11). This will be discussed later.

Because the potentials V depend on the K-matrices the K-matrix equations have to be solved by iterations. Each iteration defines new Hamiltonians H_0 and H'.

In another formulation of the theory one chooses $H_0 = \sum_i T_i$. The propagators are then free particle propagators and there are no V-insertions in lines, only K-insertions. One can still define a K-matrix as above to sum diagrams to the same approximation. This formulation appears to adhere to Brueckner's initial work. The difference between the two formulations is only formal and there is no difference whatsoever for nuclear matter. For finite nuclei there is a difference, how-

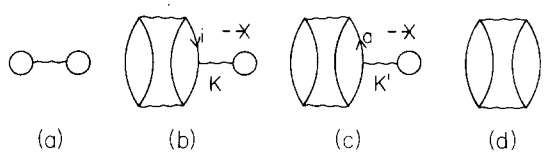

Fig. 3. Diagrams included in the nuclear matter calculation by Brueckner and Gammel [22]. Diagram (d) (and higher order ladder diagrams) is included by the definition of the K-matrix. Diagrams with any number of insertions in hole- or particle-lines are also included.

ever, and we shall return to this point in sect. 5.1.

In other developments of the theory, to be discussed in sect. 4, other diagrams are also included by redefining the potential energies V_α.

The K-matrix describes the interaction between two nucleons in the presence of the other nucleons in the nucleus. It can therefore also be regarded as a modified or effective interaction inside the nucleus. The interaction outside the nucleus is described by the scattering matrix.

In the equations above, the indices refer to model states defined by H_0. In an infinite system these are plane wave states. In a finite system they are of finite extension and the single particle or shell-model potential that defines these states will be discussed in sec. 5. If Φ denotes the *model* wave functions it is often convenient to define the *correlated* wave function Ψ by

$$\upsilon\Psi = K\Phi \,. \tag{3.15}$$

From eq. (3.11) one then finds

$$\Psi = \Phi + \Phi\frac{Q}{e}\Psi \,. \tag{3.16}$$

This equation for the two-body correlated wave function is in the literature often referred to as the Bethe–Goldstone equation [34]. The difference between the unperturbed, Φ, and the perturbed wave function, ψ,

$$\chi = \psi - \Phi \tag{3.17}$$

is referred to as the *defect* wave function. As a consequence of the *healing* [36], χ is of relative short range (in coordinate space). The *wound*-integral

$$I_w = \int |\chi|^2 \mathrm{d}r \tag{3.18}$$

is a measure of the strength of the correlations. It is often convenient to introduce a wave-operator Ω defined by

$$\psi = \Omega\Phi \,. \tag{3.19}$$

Then one also finds

$$K = \upsilon\Omega \tag{3.20}$$

and Ω is the operator that induces the correlations specific to the Brueckner theory. In the limit $\Omega = 1$ one regains the Hartree–Fock theory.

The diagrams in fig. 3 are all included in the expression (3.10) for the total energy if the K-matrix is defined by eq. (3.11). There are two important effects included by this definition of the K-matrix. The first is the *ladder summation* to infinite orders, whereby two nucleons are allowed to interact any number of times in particle states. This is accomplished by having K appear on the right hand side of eq. (3.11). The second is the *propagator modification*. This is physically motivated by the effects of other nucleons on the interaction between two nucleons propagating through the nuclear medium. By the self-consistency requirements (3.12) and (3.13) this effect is also summed to all orders. This self-consistency is referred to as Brueckner self-consistency. It is very similar to Hartree–Fock self-consistency. A formal difference is that the interaction in eq.

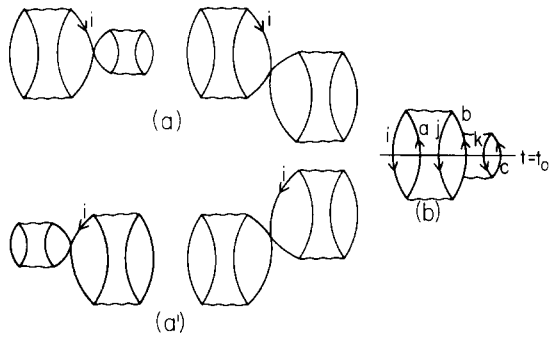

Fig. 4. Diagrams relating to the discussion of insertions in hole-lines (a) and particle-lines (b).

(3.12) is K instead of v as in eq. (2.5). More important is that the purposes of the two choices of self-consistencies are quite different. The Hartree–Fock choice is a consequence of wanting to reduce single-particle excitations. This is not at issue for nuclear matter. Brueckner self-consistency on the other hand is a consequence of a wish to reduce two-body excitations. We shall find later that to a certain approximation both aims can be achieved at the same time. We shall return to this in sect. 5.

Goldstone diagrams have been discussed at length by several other authors, for example in refs. [9, 10, 12]. We shall limit the discussion to insertions in hole- and particle-lines.

If one expands the K-matrix diagram 3b one finds the two diagrams 4a. But what about the other two diagrams 4a' which are symmetric with these two. They are distinct from the first two and should also be included. As one sums over all orbit states in diagrams 4a to calculate the total energy they will be included however and need therefore not be considered separately. They should rather be ignored to avoid overcounting. Regarding diagram 3b the terminology customarily used is to say that there is a bubble insertion in hole line i of the *skeleton*. Looking at the expanded diagrams 4a and 4a' there is an ambiguity as to which one of the two right and left symmetric parts is to be considered an insertion and which is the skeleton. A prescription is called for at this point. The rule is to choose as the skeleton that part of the diagram which is attached to the highest end of all propagator lines [9].

Particle insertions are calculated off the energy shell in eq. (3.14) as will be shown below, while hole insertions are on the energy shell. This asymmetry is a consequence of the theory and was first discussed by Brueckner [35]. It was further analyzed by Brueckner and Goldman in low order perturbation theory [37]. The proof that hole-energies should be calculated from an on the energy shell K-matrix was first given by Bethe et al. using Goldstone diagrams [32]. The point is that insertions in hole-lines can be put on the energy shell by a combination of diagrams of different time ordering as illustrated by fig. 4a. This *factorization* theorem has been derived in other many-body theories. It is only useful to apply in the case that lines cross as it is only then possible to change the relative time ordering. It is therefore not possible to apply to insertions in particle lines that therefore are to be calculated off the energy shell.

In fig. 4b the insertion in the particle line is expanded to second order. The energy denominator e' of eq. (3.14) is at $t = t_0$

$$e' = e_i + e_j + e_k - e_a - e_b - e_c \,. \tag{3.21}$$

The starting energy for calculating the K-matrix insertion in the b-line is therefore

$$\omega' = e_i + e_j + e_k - e_a \tag{3.22}$$

and the interaction between b and k depends therefore on the excitation of the other nucleons at that time. One is interested in the effect of k on the interaction between i and j. It is therefore convenient to select as the variables for treating the off-energy shell propagation

$$\begin{aligned} z_b &= e_i + e_j - e_a = \omega - e_a \\ z_a &= e_i + e_j - e_b = \omega - e_b \end{aligned} \tag{3.23}$$

where ω is the starting energy for the interaction between i and j. Equations (3.23) are coupled because

$$\begin{aligned} e_b &= e(b, z_b) = \frac{\hbar^2}{2m} b^2 + V(b, z_b) \\ V(b, z_b) &= \sum_{k<k_F} K_{bk,bk}(\omega') \end{aligned} \tag{3.24}$$

where $\omega' = z_b + e_k$. These equations relating to insertions in particle lines were first given by Brueckner and Gammel [22]. Although they apply equally well to either finite nuclei or nuclear matter they have been used only in nuclear matter calculations.

4. Nuclear matter

There are at least two reasons for studying (infinite) nuclear matter separately. Firstly, the semi-empirical mass formula contains explicitly a volume term that corresponds to the binding energy of an "infinitely" large nucleus with equal number of neutrons and protons and with the Coulomb energy neglected. Such a system is exactly what is referred to as "infinite nuclear matter" or simply "nuclear matter". Secondly, the evaluation of diagrams is in general simpler for nuclear matter than it is for finite nuclei since the wave-functions for nuclear matter are, by assumption, plane waves. One is therefore not concerned with defining the extension in space of the single particle orbitals for nuclear matter. This is on the contrary the object of Hartree–Fock theory which is applicable to atoms or weakly interacting systems. The corresponding problem for nuclei, i.e. the definition of a shell-model potential, lies actually outside the realm of Brueckner theory that primarily is concerned with correlations between nucleons. We shall come to the problem of the shell-model potential in sects. 5.2, 3. The closest counterpart to this problem is, for nuclear matter, that of the saturation density.

There is also another reason for studying nuclear matter in much detail. This is the often used "local density approximation" in finite nucleus calculations, which is based on nuclear matter calculations. This will be discussed in sect. 6.2.

We shall restrict ourselves to reviewing only a selected part of the nuclear matter problem. We shall primarily discuss some calculations dealing with insertions in hole- and particle-lines. For

further reference we refer to the review article by Bethe [13]. Most of the equations in this section as well as the comments about diagrams apply equally well to finite nuclei. The reason for reserving the material for this section is simply that it has been studied in more detail for nuclear matter.

The equations in sect. 3 relating to insertions in particle lines were simplified by Brueckner and Gammel in their nuclear matter calculations [22]. They used the approximation

$$e_k - e_c = \Delta \tag{4.1}$$

where Δ is some constant. The energy denominator e' in eq. (3.21) then becomes

$$e' = e_i + e_j - e_a - e_b + \Delta \tag{4.2}$$

i.e., it is shifted by the amount Δ relative to the energy-denominator e in eq. (3.11) referring to the interaction between i and j. Brueckner and Gammel presented calculations of the binding energy for $\Delta = 0$ and $\Delta = e_{k=k_F} - e_{k=0}$. The results seemed relatively insensitive to Δ. For the large excitations of b and k which are present especially if the nucleon force has a short ranged strong repulsion, Δ becomes quite large however and e_b then becomes large and positive. This results in a decreased attraction between the nucleons. This is clearly shown by the calculations of Coon and Dabrowski who solve the equations more accurately than the approximation implied by eq. (4.1) [38].

Large excitations of the three nucleons i, j and k in fig. 4b represent in configuration space a close collision between these three nucleons. One may therefore expect that more complicated three-body interactions than those described by diagram 4b are important. This diagram only represents a glancing interaction between k and j. The general three-body interaction necessitates the solution of the three-body problem. Bethe [39] accomplished this by using the method of Faddeyev. Day [40] made important improvements in the theory. The most complete solution to date using these methods is that of Dahlblom [41]. He used both the hard core- and the soft core Reid potentials. Dahlblom treated the off-energy shell effect approximately following a prescription of Bethe et al. [32], which tends to be good for large excitations. It was actually designed for that purpose in the belief that small excitations are relatively unimportant. For small excitations, that in configuration space corresponds to three nucleons being relatively far apart, the diagram 3c is the predominant three-body diagram. It was found by Köhler that a more exact treatment of the off-energy shell effect than that used by Dahlblom for small excitations, leads to an increase in binding of 0.7 MeV/nucleon for the Reid soft core potential [42].

Higher order Goldstone diagrams, other than those considered until now in this article have also been calculated. It lies near at hand to consider not only the first order bubble insertions in hole- and/or particle-lines, but also higher order insertions. Such insertions were first considered by Brueckner and Goldman [37] and calculations were presented in ref. [43]. They considered the second and third order insertions in hole-lines such as shown in figs. 5a, b. The second order insertion is off the energy shell here and this was approximated by an average excitation. They found the diagrams in fig. 5 to contribute 1.5 MeV/nucleon to the binding. The third order insertion $V_h^{(3)}$ is shown in fig. 6c. It is well approximated by

$$V_h^{(3)} = -\rho \cdot I_w \cdot V_h = -\kappa \cdot V_h \tag{4.3}$$

where ρ is the density, I_w the wound integral (3.18) and V_h the first order insertion shown by

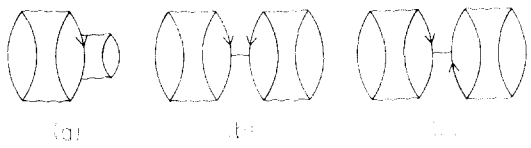

Fig. 5. Second order insertion in a hole-line (a), and a third-order insertion in hole-line (b). In the fully renormalized theory any number of third-order insertions in hole lines are included. Diagram (c) can be regarded either as an insertion in a hole-line, complementing diagram (b) or as an insertion in a particle-line complementing diagram 3c.

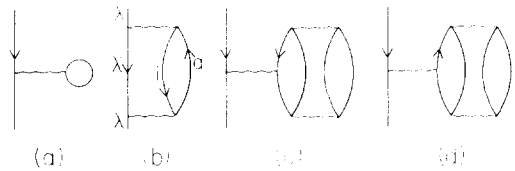

Fig. 6. Single particle energy diagrams discussed in the text.

fig. 6a, and κ is the small parameter of Brandow's [9]. This is a very useful relation. It is for example shown in refs. [44, 45]. The wound integral depends rather sensitively on the two nucleon force. It increases with increased core strength and tensor component both of which increase the correlation. Thus it is found that diagram 5b contributes about 2.0 MeV to the binding if using the hard core Hamada–Johnson potential [46] but only 1.0 MeV if one uses the Reid soft core potential [42].

Brueckner et al. find that their approximate evaluation of diagram 5a gives the same contribution from this diagram as from diagram 5b. An effort to improve upon that calculation gave a rather much smaller contribution, about 0.2 MeV/nucleon to the binding energy [42]. Brueckner et al. seem to want to conclude from their results that diagrams 5 are small and can be neglected. It may also very well be that they are smaller than many other diagrams that are neglected, but this is very hard to assert. There is, as mentioned in sect. 2, much uncertainty about the short ranged behavior of the nucleon force. It may very well be that the wound integral and therefore also diagram 5b will turn out to be smaller than calculations with present forces indicate.

It has been demonstrated, however, that diagram 5b also depends on insertions in particle lines [42, 46]. The diagram is furthermore fairly easy to calculate and these may be taken as reasons for including it in standard calculations.

Brueckner showed at an early stage of his work that the dispersion effect is important [31]. By the definition (3.11) of the K-matrix, is actually not only diagram 3b included if the energy is calculated to first order in K as in eq. (3.10). By Brueckner's definition of the K-matrix all hole-lines are "dressed by bubbles", i.e. all the diagrams with one, two, three, etc. first order K-matrix insertions in hole-lines are included. Likewise all particle-lines are dressed by bubbles, but the interactions are then off the energy shell as discussed above. Instead of calculating only diagram 5b one can also dress the hole-lines with the third order insertion 6c. This is done by including this insertion in the hole-energies e_i in eq. (3.12). This is the basis of the fully "renormalized" theory that has been very popular in the last few years. All diagrams of "type" 5b are now included if the energy is calculated by eq. (3.10) from the K-matrix with the redefined hole-energies. A cor-

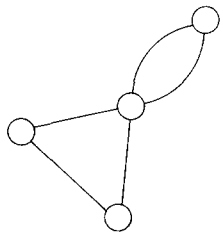

Fig. 7. An example of a Bloch diagram.

rection is however necessary because if this prescription is followed one will find that diagrams 5b due to their symmetry will be included twice. This can be done by including only half of the hole-energy calculated from diagram 6c. This was done in refs. [42, 43, 46].

For more complicated diagrams that one eventually might like to consider such a simple correction may not be possible. A general and very elegant method to treat this overcounting problem has been given by Bloch [8]. He draws a diagram using Bubbles, Lines and Cycles. An example is shown in fig. 7. The Lines represent propagators and the Bubbles are self energy insertions. Diagram 7 has four Bubbles, five Lines and two Cycles. These numbers satisfy

$$N_B - N_L + N_C = 1 \,. \tag{4.4}$$

By adding on more Bubbles and Cycles, eq. (4.4) is found to be general. By summing each diagram separately over Bubbles, Lines and Cycles and using eq. (4.4) one will count each diagram only once. Brandow applies this rule selecting the lowest order K-matrix diagrams to obtain [9]

$$E = \sum_i T_i + \tfrac{1}{2} \sum_{ij} K^{(r)}_{ij,ij} P_i P_j + \sum_i (1 - P_i) V_i \tag{4.5}$$

where

$$V_i = \sum_j K^{(r)}_{ij,ij} \cdot P_j, \qquad P_i = \left(1 + \sum_j I^{(j)}_w P_j\right)^{-1} \tag{4.6}$$

where $I^{(j)}_w$ is the wound integral (3.18) for state j. The K-matrix is now defined not with the potential energies in eq. (3.12) but with the "renormalized" energies in eq. (4.6). By expanding the energy (4.5) in small values of I_w one finds [9]

$$E = \sum_i T_i + \tfrac{1}{2} \sum_{ij} K_{ij,ij} + \tfrac{1}{2} \rho^2 I_w^2 \sum_{ij} K_{ij,ij} \tag{4.7}$$

where I_w is the wound integral $I^{(i)}_w$ averaged over states i, and the K-matrix is now defined with the potential energies in eq. (3.12). The last term in eq. (4.7) represents the diagram 5b. The difference between expressions (4.5) and (4.7) is that by the former expression, not only that particular diagram but also multiple third order insertions are included, with an overcounting correction. Köhler has shown that the contributions of diagram 5b is quite sensitively coupled to diagram 3c,

Table 1 *

Diagram	Binding energy (MeV)
3b	11.4
3b + 5b	12.2
3b + 3c	12.9
3b + 3c + 5b	15.0
3b + 3c + 5c	12.4
3b + 3c + 5b + 5c	14.0
3b + 3c + 5b + 5c **	13.6

$k_F = 1.4\ F^{-1}$; $V_a = 0$ for $k_a > 2.8\ F^{-1}$ (fig. 3c).

* This is table 1 of ref. [42].

** Calculated to all orders, fully renormalized.

i.e., to the inclusion of the particle potential energies in eq. (3.13) when defining the K-matrix [42]. Table 1 is a summary of calculations with the Reid soft core potential taken from ref. [42]. It shows that diagram 5b contributes 0.8 MeV/nucleon to the binding if the K-matrix is defined with $V_a \equiv 0$ but the same diagram contributes 2.1 MeV/nucleon if the K-matrix is defined to include diagram 3c, i.e., with a $V_a \neq 0$ and calculated from off the energy shell K-matrix insertions according to eqs. (3.21)–(3.24). Renormalizing the particle potential energies by inclusion of the diagram 5c in the K-matrix definition reduces the contribution from diagram 5b to 1.6 MeV/nucleon. By finally calculating diagram 5b in a fully renormalized theory reduces it further to 1.2 MeV/nucleon.

The conclusion to be drawn from the results summarized in table 1 and from the results of the three-body contributions [41, 42] is that the coupling between diagrams can be very important. It may also be expressed by saying that the corresponding higher order diagrams are important. It should also be pointed out that the saturation also is much affected by the higher order diagrams discussed above [42]. This can easily be understood because they are four-body diagrams and therefore proportional to the third power of the density.

The calculations of ref. [42] with the Reid soft core potential gave a binding energy of 16.7–17.3 MeV/nucleon and a saturation at $k_F \sim 1.5\ F^{-1}$. Due to the uncertainty of contributions of higher order diagrams one cannot hope to calculate the total binding energy per nucleon better than to within ±1 MeV, and the saturation fermi-momentum better than to within several tenths of 1 F^{-1}. The present uncertainties in the nucleon force may lead to similar errors. The results for the Reid soft core potential indicate that a slightly harder core repulsion (or a velocity-dependent force) would give better agreement with an experimental binding of 15.7 MeV [47], and a saturation at a lower density. The potential of Green and Haapakoski has features that suggest qualitative improvements [48].

5. Theory of finite nuclei

The theory for finite nuclei can be separated into two distinct parts, the K-matrix theory for finite nuclei and the theory of the shell model potential. There are essentially two many-body theoretical definitions of the shell-model potential to be found in the literature, the diagrammatic

and the variational. We shall discuss these separately. The concept of a shell-model potential has perhaps been the single most important concept in nuclear theory. The coherent potential (3.3) defined by Brueckner promised to be at least closely related to this shell model potential. Considerable effort has since been made to define such a potential rigorously, from a many-body theoretical point of view.

5.1. Reaction matrix for finite nuclei

The Brueckner many-body theory, the K-matrix theory, is in itself not any different for finite nuclei from what it is for infinite nuclear matter. The Goldstone expansion is valid for any choice of basis set, be it plane waves or finitely extended waves. In general one should expect that the diagrams which have been found to be important for nuclear matter calculations are also important for finite nuclei. In addition there are for finite nuclei single particle excitation diagrams that do not occur in nuclear matter theory because of momentum conservation. These are important diagrams and will be discussed below in sects. 5.2 and 5.3.

In the case of the electron many-body system one knows that specific finite size effects also are important. This was discussed in sect. 1. Whether a similar situation exists for nuclei is not yet known.

Discussing nuclear matter in sect. 4 it was pointed out that by different definitions of the K-matrix, different sets of diagrams are included when one calculates the total energy to first order in the particular K that is chosen. The same situation occurs for finite nuclei and we shall make use of this when we define the K-matrix for this case.

Typical diagrams that contribute to the total energy of a finite nucleus are shown in figs. 8 and 9. Those in fig. 9 contain single particle excitations and are specific to the finiteness of the system. Some of those in fig. 8, namely those that have diagonal hole and particle insertions, also contribute to the energy of nuclear matter. In this section we shall mainly be concerned with the diagrams in fig. 8.

The diagrams are defined by the zero-order Hamiltonian H_0 in eq. (2.2), that determines the propagators and the basis set, and by a reaction matrix K that determines the interaction. In what follows we shall refer to the potential V in eq. (2.2) as the shell-model potential U_{SM}. In subsections that follow we shall seek to define U_{SM}. Once U_{SM} is defined a reaction matrix is defined by eq. (3.11) with potential energies ($U \equiv U_{\mathrm{SM}}$)

$$V_\alpha = U_\alpha . \tag{5.1}$$

We shall later refer to this reaction matrix as K_0. In a similar fashion we can define a matrix K_0' as in eq. (3.14).

Assume now that U_{SM} is defined similarly to V_{HF} in eq. (2.5) but with v replaced by K_0 and K_0'.

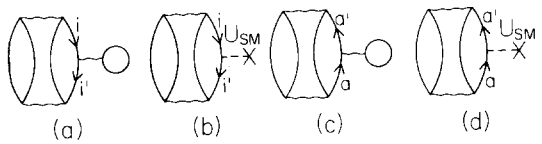

Fig. 8. Diagrams discussed in relation to the definition of the K-matrix by eq. (5.2).

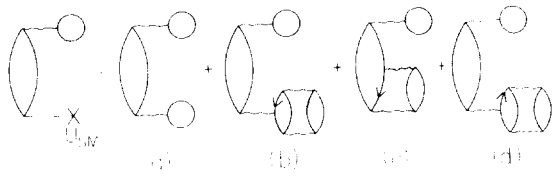

Fig. 9. By defining the particle–hole matrix elements of the shell-model potential U_{SM} as the sum of the vertex insertions 9(a)–(d), all diagrams in this figure will cancel.

This choice of U_{SM} will be discussed again in sections that follow and will be referred to as the Brueckner–Hartree–Fock (BHF) choice. The shell-model potential also serves to define wave functions. Although U_{BHF} leads to the cancellation of the diagrams 8, which we know to be important from nuclear matter studies, it does not guarantee that this potential gives the "best" definition of single particle wave functions. One is in fact often faced with a situation where one likes to generate the wave functions by some other (e.g. harmonic oscillator) potential chosen for convenience of calculation. Although the wave functions of that potential are "good", the eigenvalues may not be good enough for the purpose of cancelling diagrams 8. The energy calculated from the expression (3.10) with the reaction matrix K_0 does then in general not include diagrams 8. These are dispersion type diagrams, the importance of which Brueckner emphasized in his early work [31]. Although the definition K_0 of the reaction matrix that was obtained from eq. (5.1), has been used by many authors, it is not the best choice. It is better to choose a reaction matrix K defined by eq. (3.11) with [49]

$$V_i = \sum_j K_{ij,ij} \tag{5.2}$$

and calculate the energy (3.10) with this K. This way one sums the diagrams 8a and 8b with *diagonal* insertions ($i = i'$). It should be observed that the unperturbed Hamiltonian H_0 is not changed and the diagrams are still K_0-matrix diagrams.

Likewise, one sums diagrams 8c and 8d by

$$V_a = \sum_j K'_{aj,aj}.$$

It has sometimes been argued that it is a good approximation to neglect K-matrix insertions in particle lines. (The results for nuclear matter that is shown in sect. 4, does not support this view.) But one still has to calculate diagram 8d. This diagram will be summed by defining the matrix K with kinetic energies only in particle states, i.e. with $V_a = 0$. This has been done in many calculations. It can be refined somewhat. The kinetic energy operator is not diagonal for the shell-model states. In order to preserve the distinction between particles and holes one should, according to Baranger [50], also replace T_a by QT_aQ in eq. (3.11). Brandow [10], on the other hand, finds that the replacement of Q/e by $Q(1/e)Q$, which was first used by Wong [51], is the correct procedure to use. The effect of the refinement is anyway small [52]. The reason for this can be traced

back to the short range of the two-body correlations compared to the thickness of the nuclear surface.

The consequence of the definition (5.2) for hole energies and the similar definition for particle energies is that the choice of U_{SM} is less important as a tool to improve the convergence of diagrams representing *two*-body excitations than if one adheres to the definition (5.1). Diagrams with diagonal insertions in hole- and all insertions in particle-lines can always be summed by calculating the energy to first order in K, irrespective of U_{SM}. This is very important in practice if one performs a calculation with shell-model states defined by some potential U_{SM} which gives adequate wave functions but bad eigenvalues. An example of such a potential is the widely used harmonic oscillator potential. This implies that the off-diagonal matrix-elements of the potential are adequate but the diagonal are not.

It should also be noted that there are no off-diagonal insertions for nuclear matter, as a consequence of momentum conservation. The choice of potential spectrum is therefore of no importance whatsoever for that case. Insertions in hole and particle lines are summed by the proper definition of potential energies in the K-matrix single particle energies (see sect. 3).

In the discussion above only the first order K-matrix insertion was included as exhibited by eq. (5.2). Higher order insertions of the type discussed in sect. 4 on nuclear matter, are also includable by proper definition of the potential energies in the K-matrix. We shall return to this in sect. 5.2.

5.2. Shell-model potential, diagrammatic definition

Efforts to derive a theoretically fundamental shell-model (or self-consistent) potential U_{SM} are hampered by the fact that the choice of U_{SM} is irrelevant in the sense that the perturbation expansion is valid in any basis set defined by U_{SM}. For any choice of U_{SM} the energy or other observable can be calculated to any degree of accuracy by a successive calculation of diagrams (assuming that these converge). Rather than being an exact and fundamental concept we shall find that the shell-model potential can be used as a tool, albeit a very important tool for facilitating the calculation of some particular quantity.

It is important to realize that Brueckner's K-matrix theory in itself does not prescribe or- hardly even suggest any particular choice of U_{SM}. In sect. 5.1 we showed how a large class of diagrams involving two-body correlations can be summed by the choice of single particle energies in the definition of the K-matrix. These diagrams involve diagonal matrix-elements of U_{SM} and of K. One is on the other hand not able to sum diagrams involving *off*-diagonal insertions of U_{SM} and K, by a definition of the K-matrix. Such diagrams can however be eliminated by the choice of U_{SM} or to be more specific, by the off-diagonal matrix elements of U_{SM}.

It was pointed out in sect. 2 that the Hartree–Fock choice (2.5), applicable in atomic theory, reduces single particle excitations by cancelling diagrams of the type shown in fig. 1b. Similarly, one can make use of the freedom of choice of U_{SM} that was discussed above, to reduce single particle excitations in nuclear many-body calculations. Examples of such diagrams are shown in fig. 9. The first diagram, 9a, is similar to the diagram 1b, that is cancelled by the Hartree–Fock choice. An important difference is that the interaction here is a K-interaction rather than a v-interaction as in Hartree–Fock theory. The diagram 9a is cancelled by that particular definition of particle–hole matrix-elements of U_{SM}. This leaves open the choice of hole–hole and particle–particle

matrix-elements of U_{SM}. The Hartree–Fock choice is to define these by the same insertion as the particle–hole, thereby cancelling diagram 1d. While this may not be very important in atomic theory we have already repeatedly emphasized the importance of the corresponding diagrams 8a and 8b for nuclei. We have also found that these diagrams with diagonal insertions can be summed by the choice of the definition of the K-matrix. We now also find that all of these diagrams, both with diagonal and off-diagonal insertions can be eliminated by making a choice similar to the Hartree–Fock. Formally we just replace the v-interaction in the Hartree–Fock potential (2.5) by the K-interaction. The potential U_{SM} thus defined is in the literature often referred to as the Brueckner–Hartree–Fock (BHF) potential.

While the BHF-choice cancels diagrams with K-insertions in vertices, diagram 9a, as well as K-insertions in hole-lines, diagram 8a, this choice of U_{SM} will not sum diagrams 8c and 8d. The reason is that the K-insertions in particle lines should be calculated off the energy shell. The cancellation of the two-body excitation diagrams 8, as a consequence of the choice of the BHF-potential is however not of such a great importance. In sect. 5.1 it was shown that the most important class of these diagrams, can be summed through the definition of the K-matrix, especially by the choice of the energy denominator. The diagrams 8c and 8d that were not cancelled by BHF can also be summed by redefining the K-matrix as discussed in sect. 5.1.

It was found in early work of Brueckner and coworkers that it is not sufficient to define U_{SM} by BHF [53]. The second insertion, 9b, has been included in many calculations. It has been found to be important, perhaps not so much as total binding energy is concerned but more as far as saturation (nuclear radii) is concerned. Early calculations showed that neglecting this insertion yielded nuclear radii too small to be consistent with nuclear matter calculations [53]. Nuclear matter saturation is usually obtained by a variation of the density. We shall find in sect. 5.3 that this variation generates the contribution 9b if the energy is calculated from eqs. (3.10), (3.11). This is positive and therefore "helps" in saturation. Brandow therefore calls it a saturation potential [9]. This saturation potential is simply a factor κ times the BHF-potential and with the opposite sign. This is shown by eq. (4.3). It is therefore easy to include. We have so far only discussed the particle–hole definition of U_{SM} including diagrams 9b. One may very well keep the BHF definition of hole–hole and particle–particle matrix-elements. This may technically be difficult to do however, especially if one works in coordinate space. It is more straightforward to define these matrix-elements of U_{SM} by the same insertion as used for the vertex. One will then also include diagrams 5b and 5c in the expression for the total energy. These were discussed in sect. 4 on nuclear matter. Their contribution depends on the strength of the two-body correlations which in turn depends on the two-body force. Whether it is justified numerically, to include these diagrams can therefore not be firmly established as yet. Making these insertions in hole and particle lines one runs into a problem of overcounting already shown in sect. 4. This can be resolved by calculating the energy, not from eq. (3.10) but from eq. (4.5). The ensuing theory is usually referred to as the Renormalized Brueckner–Hartree–Fock theory or RBHF.

The insertion 9c is technically more difficult to handle. Not many calculations have therefore been made including this insertion and its importance has not been fully established. One should note that the similar insertion in hole-lines shown by diagram 5a is off the energy shell and therefore much smaller, as was found in sect. 4. It can therefore be neglected.

In the calculations of Masterson and Lockett [54] and of Köhler [55], the diagram 6b was calculated for nuclear matter and then used as an approximation for the insertion in 9c. These cal-

Fig. 10. The energy diagram 9c is small. As an alternative way of calculating the corresponding effect on density distribution one can calculate the diagram above.

culations show that the insertion 9c mainly affects single particle wavefunctions while total binding energy is only slightly affected. For this reason and because it is complicated to calculate one can consider neglecting this insertion. To find the effect on the nuclear radius as a consequence of the change in wavefunctions one can instead calculate diagram 10. One may of course also explicitly calculate the corresponding energy diagram. One may likewise consider calculating the effect of the insertion 9b on the nuclear radius. But this insertion is so easy to include anyway, that such a procedure would not be a simplification of calculations. We shall return to these matters especially in sect. 6.

5.3. Shell-model potential, variational definition

It is well known that the Hartree–Fock definition (2.5) of a self-consistent potential can be derived by the Rayleigh–Ritz variational principle. Correlations between particles are neglected in this theory. Löwdin formulates an Exact Self-Consistent Field Theory (ESCF) in which correlations are included to all orders [56]. This theory has been shown by Kobe [57] to be equivalent to a proposal by Brenig [58]. Brenig defines the "best" single particle-orbitals as those having the maximum overlap with the true wavefunction. At least in its exact form this ESCF-theory is too complicated to apply to nuclei. We still wish to briefly review this theory as we think it illuminates some points in the Brueckner reaction matrix theory.

Let the exact Hamiltonian (2.1) satisfy

$$H\psi = E\psi \tag{5.3}$$

and let ϕ_0 be a Slater determinant satisfying

$$H_0\,\phi_0 = E_0\,\phi_0\,. \tag{5.4}$$

The aim is to find the "best" ϕ_0. Löwdin defines an *exact* reaction operator t by

$$t\phi_0 = V\psi \tag{5.5}$$

where V is the perturbation, denoted H' in eq. (2.4). It thus includes the one-body operators V_i. The eq. (5.5) is only formally similar to eq. (3.15) which refers to the Brueckner K-matrix. In the latter equation v is the two-body force and the wavefunction is a two-body correlated wavefunction. The potential V in eq. (5.5) includes the one-body potentials V_i (see eq. (2.4)) and the wavefunction is the total many body wavefunction. If

$$\langle\psi|\phi_0\rangle = 1 \tag{5.6}$$

one finds that the exact ground state energy is given by

$$E = \langle \phi_0 | H_0 + t | \phi_0 \rangle . \tag{5.7}$$

This result is actually just a reformulation of the exact eigenvalue problem (5.3). It implies a complete summation of the perturbation series, if convergent. It is valid for any choice of ϕ_0. The reaction operator t satisfies a Lippman–Schwinger type equation [59], like the Brueckner reaction operator K does, eq. (3.11). Diagrammatically, t includes all diagrams while K only selects those that are considered important. It is especially to be noted that t includes single particle excitations while K includes primarily two-body excitations. Like the K operator, t also depends, through its definition, on the chosen basis set ϕ_0.

The expression (5.7) being exact can not be improved by variation [44]. This is an important difference from the Hartree–Fock scheme which of course is approximate. Evidently intrigued by the usefulness of the Hartree–Fock iteration scheme Löwdin performs a variation *neglecting the dependence of t upon* ϕ_0. This variation forms the basis of his ESCF-theory. The variation is assumed to give some minimum $E_{\min}$, but $E_{\min}$ may be larger or smaller than the exact E because this is not a Rayleigh–Ritz variation [57]. The method (probably) defines some one body potential and as eq. (5.7) is exact for any ϕ_0 one can use the orbitals ϕ defined by this potential to calculate the exact energy E. The potential which is found by this method will of course depend upon the orbitals, say χ, for which t is calculated so that ϕ are functionals of χ,

$$\phi = \phi(\chi) . \tag{5.8}$$

If one can reach a situation such that

$$\phi(\chi) = \chi \tag{5.9}$$

after the variation has been performed, then $E_{\min} = E$. Kobe therefore proposes to impose the relation (5.9) as a subsidiary condition [57]. This would lead to a unique Self Consistent Field (SCF) potential and a unique energy minimum equal to the exact ground state energy. Meldner and Perez have questioned how the condition (5.9) can be reached in practice by the iterations [60].

The Hartree–Fock orbitals ϕ_0 defined by eq. (2.5) satisfy the so-called Brillouin condition [61]

$$\langle \phi_0 | H' | \phi_{\text{s.e.}} \rangle = 0 \tag{5.10}$$

where $\phi_{\text{s.e.}}$ denotes a singly excited function. The condition (5.10) expresses the same property of the Hartree–Fock choice that was discussed in sect. 5.2. It was there formulated as a reduction of the single-particle excitation diagrams. Likewise the orbitals (5.8) and the exact reaction matrix $t(\chi)$ satisfy

$$\langle \phi_0 | t | \phi_{\text{s.e.}} \rangle = 0 . \tag{5.11}$$

Löwdin calls this the Brillouin–Brueckner theorem. Diagrammatically one would thus say that the potential defined by the ESCF-theory minimizes the single particle excitation diagrams, which was also the purpose of the choice of the potential U_{SM} in sect. 5.2.

Brenig proposed to define the orbitals ϕ_0 by

$$\langle \psi | \phi_0 \rangle = \max \tag{5.12}$$

where ψ is the exact wavefunction (5.3). Kobe has shown that the condition (5.12) is satisfied by the ESCF orbitals [57]. Introducing the wave operator Ω by

$$\psi = \Omega\phi_0 \tag{5.13}$$

one also finds [44]

$$\Omega = 1 + G_0 t \,. \tag{5.14}$$

Varying ϕ_0 in eq. (5.12) one finds

$$\langle\psi|\phi_{\text{s.e.}}\rangle = 0 \tag{5.15}$$

i.e. the orbitals defined by eq. (5.12) satisfy the condition that the singly excited configurations have no overlap with the true ground state wave function. Substituting eqs. (5.13), (5.14) into eq. (5.15) one finds eq. (5.11). The ESCF-orbitals have therefore the very attractive property of minimizing single particle excitations and also satisfy the maximum overlap criterion.

One first impression of this theory is that it contradicts the diagrammatic result in sect. 5.2 where not only diagram 9a but also diagrams 9b and 9c contribute to single particle excitations. If t is replaced in the ESCF-theory by K the theory suggests that the insertions 9b and 9c should not be included in the single particle potential defined to reduce single particle excitations. On the contrary it would seem that Kobe has shown that the first order K-matrix insertion alone would reduce such excitations. This result is in appearance only however. The reaction operator t defined by Löwdin is *exact* and includes multiple particle correlations while the reaction operator K is a two-body operator, although some effects of other nucleons on the two body interaction is allowed for. The insertion in diagram 9b for example involves three nucleons. It cannot be included in a two-body operator e.g. in K but is included in t as this is the exact operator including all many particle correlations.

The question whether the higher order insertions discussed above (sometimes referred to as "rearrangement" corrections although that is often misleading) should be included or not in the definition of the shell model potential has been much discussed in the literature. The disagreements that have existed about this question are mostly related to the definition of the reaction operator [60, 62, 63]. In the definition of the K-matrix used here they definitely do occur. They do not occur for the exact t-matrix. The differences occurring between the variations of a full and restricted hole-line expansion is also emphasized by Schäfer and Weidenmüller [64].

Variational principles have been used for the definition of the shell model potential in many applications of Brueckner theory. The use of this principle in Brueckner theory has often been termed as unjustified. In calculations on nuclear matter, sect. 4, one customarily calculates the energy at different densities and the density of nuclear matter (saturation density) is chosen to be the density at minimum energy. One is not directly concerned with calculating a shell model potential here as the orbitals always are (by assumption) plane waves. The method nevertheless implies a variational principle. The variation involves the change in some external parameters that compress or expand the "infinite" piece of nuclear matter. The method is justified by a thermodynamic argument. The equilibrium of a zero temperature system is found at the minimum energy. The non-equilibrium conditions correspond to the system under the influence of constraints. It is important to realize that the Brueckner method also allows us to calculate the energy away from equilibrium, i.e., subject to compression or expansion. This is done by calculating the K-matrix by

eq. (3.11) at each density with the Q operator and energy denominator appropriate to that density.

In the first application of Brueckner theory to finite nuclei [53] a variational principle was used on the energy [65, 66] to derive the shell model potential. The K-matrix was calculated by a Local Density Approximation (LDA). This is also reviewed in sect. 6.2. The total energy which was varied was then obtained from

$$E = \sum_i \langle \phi_i | T | \phi_i \rangle + \tfrac{1}{2} \sum_{ij} \langle \phi_i \phi_j | K(\rho) | \phi_i \phi_j \rangle \, . \tag{5.16}$$

The density ρ depends on the orbits ϕ and the variation of this ρ was performed in addition to the variation of the explicit ϕ's in eq. (5.16). The latter variation gives a contribution to the shell model potential corresponding to the insertion 9a. The former variation gives a contribution that was called a "rearrangement" term [66]. Although this term is similar to the true rearrangement term discussed in sect. 7 this nomenclature is misleading in this connection and should be avoided. Rather it corresponds to the insertions 9b and 9c. It was found to be numerically important and contribute to the saturation. One must realize that the variation performed here is not a Rayleigh–Ritz variation [9]. The ϕ's in eq. (5.16) are not trial wave functions as is required for this principle to be applicable. The method can however be justified otherwise.

It is actually very similar to the variation used in nuclear matter calculations that was described above. The variational parameters in eq. (5.16) are the ϕ's while in nuclear matter there is only one parameter, the density. The $K(\rho)$ in eq. (5.16) is found from nuclear matter calculations. There is a one-to-one correspondence between density and the ϕ's if $\rho(r) = \sum_i |\phi_i(r)|^2$ i.e., if higher order corrections to the density are neglected. Although the variation is done with respect to ρ, it could equally well be done with respect to ϕ. According to Hohenberg and Kohn [67] there exists for a many body system a unique energy functional $E[\rho(r)]$ with a minimum value for some $\rho(r)$ corresponding to the ground state. The expression (5.16) can be regarded as this energy functional. It should be noted however that this theory does not justify the LDA. It seems as if this theory is similar to the external variable variation discussed above for nuclear matter.

The variation of the energy (5.16) can also be justified diagrammatically. It was noted below this equation that the variations generate the insertions 9a–c. This statement should perhaps be clarified. The K-matrix depends on the Pauli operator and on the energy denominator. If one varies the wave functions in the expression (3.10) for the energy with the K-matrix given by eq. (3.11), (thus including the diagrams in fig. 3) this variation generates:

i) Diagram 9a from diagram 3a.
ii) Diagram 9b from diagram 3b.
iii) Diagram 9c from diagram 3d.
iv) Diagram 9d from diagram 3c.

Diagram 9a is similar to the Hartree–Fock diagram and is generated by the wave functions bracketing the K-matrix. The other diagrams are generated because the K-matrix itself also depends on the wave functions.

It should here especially be observed that we have started with an energy expression that does *not* include the third order insertion in hole-lines shown in diagrams 5b. But the variation yields a definition of U_{SM} that includes the third order insertion at a vertex shown in diagram 9b. That

might seem inconsistent but it really is not. The point is that the insertion 9b is part in determining the wave functions, i.e. the radii (or saturation). It has been found relatively more important in that role than as an insertion in hole lines for calculation of the total energy shown by diagram 5b.

Another reason for keeping the insertion 9b but neglecting diagram 5b, is for consistency with most nuclear matter calculations, in which the energy is calculated with first order K-matrix insertions only in lines. In other words, diagrams 3 are included in the energy. The saturation density is found from the minimum of the energy-density curve obtained from allowing the K-matrix to depend on the density both in the Pauli operator and in the energy denominator. Then, this nuclear matter calculation is consistent with a finite nucleus calculation in which insertion 9b is kept, but not diagram 5b is included. There has apparently been some confusion about these points in the literature in relation to the renormalized theory. In this theory the third order insertion is included everywhere. One point to observe is that diagram 3a is already the lowest order renormalization diagram, diagram 5b being the next order. Another point to observe is that the insertion at a vertex determines the wave functions while the insertion in a line determines a single particle energy of the nucleon propagating through the nucleus. These are physically two different effects.

It is the dependence of K on the wave functions that is approximated by a *density* dependence of the K-matrix in eq. (5.16). Such an approximation is evidently justified in nuclear matter where the Pauli operator and the energy denominator both *are* dependent on the density, which is the only structure dependent parameter. In finite nuclei the K-matrix dependence on local density alone, is evidently an approximation. We refer to it as LDA. The contributions to the shell-model potential that come from the variation of the density ρ in the $K(\rho)$ in eq. (5.16) can therefore be regarded as approximations to the insertions in diagrams 9b–d. This seems also to have been the interpretation of Brueckner and Goldman [37, 66]. This point is also discussed below and in sect. 6.2.

Many finite nucleus calculations have been done with U_{SM} chosen to be a harmonic oscillator potential. This gives good approximations to the wave functions for small nuclei, like ^{16}O. The oscillator frequency is then varied to find the minimum energy in order to obtain the binding-energy and the single particle wave functions [68–72]. (See also ref. [13] for further references.) For this procedure to be justified it is necessary that the K-matrix is calculated with potential energies given by eq. (5.2) and not by eq. (5.1). We repeat here the statement given previously: This variation of the energy calculated from eqs. (3.10)–(3.12) is consistent with keeping all the insertions in diagrams 9 when one makes a self-consistent field calculation.

In accordance with our discussions in sect. 5.1, the above procedure, varying the oscillator frequency, implies a calculation of the energy as a function of an external parameter. The variation of this frequency parameter leads to a variation of the density, although restrained, and can therefore also be considered as a variation of that latter quantity. The thermodynamic argument mentioned in the beginning of this section *or* the Hohenberg–Kohn theorem [67] therefore justifies the selection of the energy minimum as giving the ground state.

To be consistent one should not calculate the density from the model wave function ϕ but from the correlated wave function ψ, given by eq. (3.19). This complication does not exist for nuclear matter, of course. It is also mostly ignored for finite nuclei. If the energy is calculated from eq. (3.10) the corresponding wave operator Ω is a two-body operator of relatively short

range in coordinate space. The difference between densities calculated from ψ or from ϕ is then relatively small but it can be calculated [68, 73]. If higher order diagrams have to be included in the approximation to the energy, the difference can become important. This would for example be the case if the shell model potential U_{SM} is chosen so that single particle excitation diagrams are important. The corresponding Ω then involves single particle excitations when operating on ϕ and significant corrections to the density can result. This is related to the fact, mentioned in the beginning of this section, that the calculated energy and the density distribution both are independent of the basis set if sufficient number of diagrams, and especially single particle excitations diagrams, are included. On the other hand, these diagrams can be minimized by choosing the self-consistent basis set, defining U_{SM} by the diagrams in fig. 9.

For our discussion of the variation of the energy with respect to density it is important that *if* single particle excitation diagrams are included in the energy which is varied, the density should also be calculated with the Ω-operator corresponding to these diagrams. This can become quite complicated however. It is therefore best to omit these diagrams. This conclusion was also reached by Brandow [9]. They can be calculated after the variation has been performed and the energy minimum found. If they are not small at this minimum the shell-model potential would have to be improved upon *or* one might as an alternative actually calculate the corresponding correction to the density distribution.

The one parameter variational principle for the harmonic oscillator potential can be extended to a several parameter variation. In atomic Hartree–Fock theory the general variation of the wave functions (corresponding to an infinite number of parameters) generates the Hartree–Fock potential, i.e., the insertion 9a. The variation of the energy calculated from the Brueckner-expression (3.10) generates the insertion 9a *and* also insertions 9b and 9c. Insertion 9b is generated because the K-matrix (3.11) depends on starting energies (3.13), and insertion 9c because of the Q-operator in the K-matrix.

A variation definition of the shell model potential was suggested by Köhler [74]. Similar definitions have been discussed by Brandow [9] and by Kirson [75], but they differ from the one presented here in important respects. Brandow requires that the K-matrix (3.11) is defined with single particle energies (3.12) and (3.13) equal to the energy-eigenvalues given by the shell model potential, i.e. he requires eq. (5.1) to be satisfied. Köhler's K-matrix is on the other hand defined by eq. (5.2) instead of eq. (5.1). This is an important difference as was pointed out in sec. 5.1. Kirson treats the single particle energies in the K-matrix as free parameters. This does not lead to any definition of a shell model potential as Kirson also notes.

It was pointed out above that the variation of the expression (5.16) is not a Rayleigh–Ritz variation. The variation of the Brueckner energy (3.10) that we have just discussed is not an application of this principle either. It can however be *a priori* justified as a variation with respect to external parameters just as for the harmonic oscillator representation. Important is also the *a posteriori* finding that the variation generates the diagrams in fig. 9, i.e., it defines orbitals such that single particle excitations become minimized. Eq. (5.15) is then approximately satisfied.

The diagrams in fig. 9 are also implicitly generated when making variations with respect to a finite number of parameters. It should especially be noted that diagram 9c will be generated. This diagram contributes a positive term to the shell model potential and thus increases nuclear radii. This diagram is usually not included in the definition of the shell-model potential U_{SM}. We discussed this in sect. 5.2. The variational calculation of Coon emphasizes this difference [76]. It

would be important to realize this if one considers calculating the shell-model potential for an imagined, very large ("infinite") nucleus. Then, in order to obtain the same saturation density as from the energy-density curve, calculated by a conventional nuclear matter calculation, one would have to include in the shell-model potential *all* the diagrams in fig. 9.

It is now interesting to compare the variations of the Brueckner approximation to the total energy, with Löwdin's ESCF-theory. We remind that Löwdin's theory was obtained by neglecting the dependence of the exact theory on the orbitals ϕ_0, when performing the variation. The variation of the Brueckner energy as described above can be justified both *a priori* and *a posteriori*, but there is no *a priori* justification for the Löwdin variation. It can however be *a posteriori* justified as it results in orbitals ϕ_0 with certain satisfactory properties that were discussed above.

Another point worth emphasizing is that the exact t-matrix satisfies the Brillouin–Brueckner theorem (5.11), while the K-matrix does not. It is however (approximately) satisfied by the sum of the insertions in fig. 9.

Our discussion of the variational method above was based on the Brueckner energy (3.10). The variation of the renormalized energy expression (4.5) generates the same diagrams, fig. 9, the only difference being that the interactions now are fully renormalized $K^{(r)}$-matrices, eq. (4.5), and renormalized by the factors P_i defined in eq. (4.6). Diagram 9b, being the first order renormalization of diagram 9a (cf. eq. (4.3)) is already included by the renormalization (factors P_i) and should no longer be calculated explicitly.

Brandow emphasizes that the renormalized energy (4.5) satisfies [9]

$$\partial E/\partial V_i = 0\,, \qquad \partial E/\partial P_i = 0 \tag{5.17}$$

i.e., a minimal condition is satisfied by the definitions (4.5), (4.6). This is *not* identical to the variational method used to generate the shell model potential that has been discussed previously in this section. It instead refers to an algebraic relation between E, V_i and P_i. It results from a general mass operator variational principle [8]. But it does not *define* any shell model potential. It *does* define such a potential if one also prescribes that the V_i are the potential energies of that potential. As it was stated above, the potential V_i, that is defined by eq. (4.6), includes diagram 9b but it does not include diagram 9c. If calculations are made following Brandow's prescription one can however correct for the effect of diagram 9c on the wave-functions and on the radius by calculating diagram 10. (See also sects. 5.2 and 6.1.)

If one considers insertions in particle lines (which one really should as was shown in sect. 4), one would to be consistent also have to correct for diagram 9d. It would however be simpler to include that diagram in the definition of the shell model potential.

5.4. Final remarks on the shell-model potential and on the reaction-matrix

We have discussed the shell-model potential derived by either the diagrammatic or the variational techniques. It should be apparent from these discussions that the diagrammatic definition is definitely "cleaner". The definition in terms of the variational technique is very much argumentative. It is really more intended as a justification of the calculations that have been made using this technique. The method to be used depends mostly on practical considerations. In the case that one expands the single particle states in some basis set of states and uses realistic interactions it is quite feasible to calculate the matrix elements of the shell-model potential defined diagram-

matically. This has lately been done including the second order insertion [77]. (See also sect. 6.1.) If one calculates the shell-model potential in coordinate space such an inclusion of the second order insertion is not practical. One may then instead calculate diagram 10 or use a variational technique.

We like to emphasize however that the definition of a shell-model potential is irrelevant from a *basic theoretical* point of view. The formal perturbation expansion is valid in any basis set or choice of shell-model potential U_{SM}. One may very well let the practical choice of this basis set depend on the problem one wishes to consider. Such a point of view has also been forwarded by Kirson [78]. A "fundamental" theoretical potential U_{SM} just does not exist, but U_{SM} is rather a computational aid to be chosen out of practical considerations. In previous sections this potential was discussed and defined mainly for the purpose of calculating binding energy and/or density distributions.

Another definition is due to Baranger [79]. He chooses to define a potential so that the energy eigenvalues corresponding to his potential agree with the centroid of the removal energies discussed in sect. 7.

Still another definition is due to Meldner and Perez [63, 80]. Rather than seeking agreement with the centroid of removal energies they seek to reproduce the "shifted" single particle energies including its width. The differences between the shifted and the centroid energies lies mainly in the second order rearrangement energy (fig. 6b). It is very similar to some previous definitions where the real part of the second order diagram 6b was included approximately in the shell-model potential [54, 74].

It was pointed out in sect. 5.2 that it is convenient to choose U_{SM} so as to minimize *one* particle excitations. One can likewise choose the energies e in the K-matrix equation (3.11) so as to minimize *two* particle excitations. This can be done irrespective of the choice of U_{SM} and corresponds to defining nucleon propagators through the nuclear medium that is defined by U_{SM}. It was pointed out in sect. 5.1 that the choice of hole energies given by eq. (5.2) results in the summation of diagrams 8a and 8b, with diagonal insertions which are the most important ones. This actually corresponds to the original Brueckner choice for nuclear matter for which only diagonal insertions contribute. In sect. 4 it was mentioned that Brueckner et al. also made calculations with the third order insertion in hole lines, diagram 6c. They concluded that the resulting energy diagram 5b is negligible compared to other uncertainties in the theory. The contribution of this diagram depends rather critically on the assumption made about the nucleon–nucleon force. A strong short ranged repulsion gives a larger contribution than a softer or velocity dependent repulsion. This diagram is namely proportional to I_w^2, eq. (4.7), and the wound integral I_w defined by eq. (3.18) increases with the strength of the two-body correlation. Because of the uncertainties in our knowledge of the nucleon force there is therefore also an uncertainty about the importance of this diagram. In sect. 4 we also presented results of calculations that showed that the contribution of the diagram which we discuss here, depends quite sensitively on the treatment of the off energy shell particle propagation.

It is in any case computationally relatively easy to include diagram 5b. This is done, correcting for overcounting in the renormalized theory contained in eqs. (4.5), (4.6). The third order insertion is decisively more important to include in the vertex insertion as in diagram 9b, than in the line insertion as in diagram 5b. The insertion 9b is important for saturation. To include this insertion is consistent with the calculations on nuclear matter even though diagram 5b is neglected but

the saturation is found at the energy minimum. The insertions of the third order diagram both at vertices and in lines result in RBHF-theory discussed in sect. 5.2.

Brueckner et al. also estimated the second order diagram 6b which, when inserted as in the energy diagram 5a, is off the energy shell. They found the correction to the binding to be about as large as from the third order insertion [43]. The second order insertion is technically quite hard to calculate accurately. A later estimate has shown it to be much smaller [42]. The second-order insertion at a vertex is related to the Q-dependence of the K-matrix. This insertion is generated by a variation of the wave functions that determine the Q-operator. It is also consistent with nuclear matter calculations to include this diagram in the definition of U_{SM}. In nuclear matter calculations one only varies the Fermi momentum, i.e. the wave function of the topmost state. This variation is normally not made explicitly but is made implicitly by allowing the Q-operator to depend on the Fermi momentum. In a finite nucleus all wave functions are to be varied. It has been argued that the strong momentum dependence (nonlocality) of the second order diagram 6b [43, 74], for this reason should make diagram 9c more important for finite nuclei than the corresponding diagram 6b at momentum k_F is for nuclear matter [81].

6. Calculations on finite nuclei

There are two types of calculations on finite nuclei to be found in the literature. One follows rather closely the nuclear matter calculations as presented in sect. 4. It starts from calculating a reaction matrix for some realistic two-body interaction and proceeds to calculating energy diagrams. If done in an oscillator basis this can be done with a computing accuracy comparable to that for nuclear matter. The other type of calculation starts with an effective reaction matrix sometimes more or less derived from calculations on nuclear matter with a realistic interaction. Detailed accounts of some of these calculations are found in the article by Bethe [13]. Here a few points only are discussed either because they are recent or because it is felt that they need to be illuminated.

6.1. Reaction matrix from realistic potentials

If calculations are made in a harmonic oscillator basis the energy diagrams that were discussed in some detail in connection with infinite nuclear matter in sect. 4 can be calculated with good accuracy. In sect. 5.1 it was shown how the definition of the K-matrix is related to the summation of diagrams involving insertions in hole- and particle-lines.

The experimental binding energy of the oxygen-16 nucleus is 127.6 MeV. Including the hole-insertions described by diagrams 3b and 5b but no particle-insertions the oxygen-16 binding is found to be 68.0 MeV [52] with the Reid Soft Core potential. This seems an appreciable underbinding. However this is to be expected from the corresponding nuclear matter calculation. From table 1 one finds that this calculation yields 12.2 MeV/nucleon or in other words, the *volume* energy is found to be ~3.5 MeV/nucleon too small if the same diagrams are considered. If one corrected for this discrepancy one would gain ~56 MeV for oxygen-16 to give ~124 MeV binding in close agreement with the experimental value. Of course one would also expect some change in surface energy etc. depending on how the correction was done. Our estimate here only serves to

illustrate an obvious but often overlooked consistency between nuclear matter and finite nucleus calculations.

A similar estimate can be done for lead-208. The experimental binding of this nucleus is 1636 MeV. The result of the calculations similar to those for oxygen-16 which were quoted above is 720 MeV. Correcting for the error in volume energy one finds an increase in binding to 1448 MeV in much better agreement with experiment.

It has been shown [42] that an improved volume energy is obtained by also considering insertions in particle lines (see table 1). These are numerically somewhat more difficult to do for finite nuclei. Approximate inclusion of these insertions have been done by shifting the particle spectra in the harmonic oscillator basis [52]. Those calculations are very inconclusive however and really only show the obvious that the binding is increased by shifting the particle spectrum down, i.e. by reducing the difference between hole- and particle-energies.

Even more difficult may the subject of saturation be, i.e. the problem of the nuclear radius. It is found that insertions in particle lines increase the saturation density of nuclear matter appreciably [42] and calculations on finite nuclei without these insertions already tend to give too small radii. When including insertions in particle-lines one should, to be consistent, also include the diagram 9d in the shell model potential. It is not quite evident if this contributes positively or negatively i.e., if it would offset or enhance the decrease in nuclear radius from the more attractive K-matrix calculated with insertions in particle-lines. There are both negative and positive contributions and the net result depends both on the force and on the required cutoff in particle spectrum [42].

It is to be noted however that the "best" calculation including particle line insertions gave a reasonable Fermi momentum of 1.5 F^{-1}. The density of saturation was obtained by searching for the energy minimum. This calculation includes therefore (implicitly), as was explained in sect. 5.3, *all* the shell-model insertions of fig. 9. Most finite nucleus calculations have completely ignored diagram 9c or the equivalent diagram 10. The calculations that have considered either of these diagrams indicate an increase of some 0.1 F in the nuclear radius. Diagram 9c has explicitly been included only very approximately (see sects. 5.2 and 6.2). It is included implicitly in the variational calculations of Coon [76] (see sect. 5.1). Diagram 10 has been calculated with v-interactions using the Tabakin potential [20].

A recent calculation on ^{16}O of Rouben, Padjen and Saunier [77] includes the second order insertion both in the vertex, fig. 9c, and in the hole line, fig. 5a. They find that these insertions (actually the vertex insertion) increases the radius by ~0.1 F while the total binding is increased by 3–5 MeV, thus in qualitative agreement with previous estimates. Similar increase in the radius is reported by Tripathi, Faessler and MacKellar [82].

A calculation of the binding energy of nuclear matter with the Reid Soft Core potential yields a saturation density at $k_F = 1.44$ F^{-1}, if no insertions in particle lines are included [42]. This calculation was repeated but this time suppressing the change of the Q-operator with density. It was then found that the saturation density increased to $k_F = 1.55$ F^{-1}. One would therefore expect an 8% increase in the radius of a large nucleus like ^{208}Pb, from including the second order insertion at the vertex. One should however also expect that this effect would depend on simultaneous insertions in particle lines. These matters have not yet been fully investigated.

The least understood problem of finite nuclei is probably that of the spin–orbit splitting for spin-unsaturated orbits. On the other hand, it is remarkable that the simple spin–orbit potential

$$V_{LS} = \alpha \frac{\hbar^2}{2M^2C^2} \frac{1}{r} \frac{dV_C}{dr} L \cdot S \tag{6.1}$$

where V_C is the central field gives excellent agreement with spin–orbit splittings for a value of $\alpha \approx 30$ [83]. This value of α agrees well with that found when using an optical model description of nucleons scattered by nuclei.

We have noted that there are diagrams which have been calculated for nuclear matter but which still have to be calculated for finite nuclei. It may very well be that there are also explicit "finite nucleus diagrams" (other than the obvious single particle excitation diagrams removed by the choice of U_{SM}) due to surface or collective effects. These would probably be rather complicated to calculate. But they would also probably be due to long ranged correlations as the short ranged correlations should be absorbed in the K-matrix. There could also very well be many-body correlations. An alternative to calculating these diagrams explicitly would be a standard shell model calculation in the space immediately above the Fermi level. The rest of the space would be included by the K-matrix. A calculation of this type has been made for helium-4 [84]. It yielded a relatively small correction. It is believed however that these contributions are rather sensitive to the exact treatment of the particle spectrum and that was not done in ref. [84]. The small "gap" that really does exist in the spectrum close to the Fermi-surface could induce important correlations.

6.2. Reaction matrix from semiphenomenological theory

Due to the comparative ease with which nuclear matter calculations can be made it is compelling to somehow use such results for calculations on finite nuclei. This is a procedure also used in atomic physics to different degrees of sophistication. As examples we mention the Thomas–Fermi theory and the Kohn–Sham method [67, 85]. Similar methods have been used in the finite nucleus calculations of Bethe et al. [86], Brueckner et al. [87], Myers and Swiatecki [88] and others.

An approach using a similar idea but somewhat different in execution was first taken in the calculations of Brueckner, Lockett and Rotenberg [53]. In a finite nucleus calculation a major problem is the computation of the reaction matrix in the finite geometry (unless one uses Harmonic Oscillator wave-functions). Brueckner et al. circumvented this problem by approximating the reaction matrix in the finite nucleus by a Local Density Approximation (LDA) that was also discussed in sect. 5.3. They used the approximation [65] (see also eq. (5.16))

$$\langle ij|K|ij\rangle \simeq \langle ij|K_{NM}(\rho)|ij\rangle \tag{6.2}$$

where ρ is the density at the center of mass point of the two interacting nucleons and $K_{NM}(\rho)$ is the nuclear matter reaction matrix at that density. It was furthermore assumed that only the short ranged part of the reaction matrix is density dependent. This assumption was based on numerical estimates. The results of these calculations were considered as somewhat discouraging. The calculations gave the right binding energy for nuclear matter, but the finite nucleus K-matrix derived from these calculations gave too small binding energies for light nuclei. This may be described as a failure of the theory to give the correct surface energy. One can consider two possible reasons for the failure. Firstly, the LDA is perhaps inadequate and secondly, other diagrams than those considered for nuclear matter may be important for finite nuclei. The second possibility is far

more difficult to investigate. It was discussed shortly in sect. 6.1. On the other hand there have been discovered errors in the LDA as used by Brueckner et al. Köhler pointed out, that although these authors concluded that the density dependence stems from the short ranged part of the interaction, the results they present indicate a non-negligible dependence of the *long* ranged part [74]. This can be traced to the tensor component of the force. It was also pointed out by Köhler [44] that the LDA is incapable of correctly treating the dispersion-effect i.e., the dependence on starting energies. He showed that a better treatment of this effect increases the binding of oxygen-16 by 2.5 MeV/nucleon, while for calcium-40 the increase is 2.2 MeV [55].

Brueckner et al. defined their shell model potential by variation as shown in sect. 5.3. The density dependence of the K-matrix generates contributions to this potential ("rearrangement potentials") that are local, while the exact theory shows that these contributions are non-local. This is also seen explicitly from the nuclear matter work by Brueckner et al. [43]. Masterson and Lockett incorporated this non-local effect in their finite nucleus calculations [54]. This also amounted to an approximate inclusion of the insertion 9c in the definition of the shell model potential as discussed in sect. 5.2. The most striking result of this non-locality is, of course, that the energy eigenvalues become much more negative. A similar effect has been investigated later by Lin and Köhler [89].

The calculations of Negele [90] have been reviewed by Bethe [13]. He also uses a LDA but following Köhler he allows for a dependence on starting energies and his density dependence is not restricted to the short ranged part of the interaction. In these respects his calculations are improvements over those of Brueckner et al., but Negele approximates part of the non-locality of the K-matrix by a density dependence while Brueckner et al. treated this exactly. This can lead to errors in single particle energies [89].

Both of the calculations described involve a partial adjustment of the interaction. They are in this sense semiphenomenological theories. Even so they lead to rather complicated calculations involving the handling of K-matrices of detailed structure. But the main results of the calculations of binding energy etc. depend on the average properties of these matrices. It therefore lies near at hand to try to simplify the theory by seeking to define such an average K-matrix in such a way that data are reproduced. The approach is then in a sense similar to the development of the semi-empirical mass formula. A difference is that the parametrization now lies in the interaction rather than in the volume, surface, etc. energies. An example of such an interaction is the Skyrme-interaction used e.g. by Vautherin et al. [91]. Sprung et al. derive an interaction from calculations on nuclear matter [92]. Moszkowski et al. use a parametrized interaction [93] while Nemeth and Ripka [94] use the Negele interaction. Köhler has used the Brueckner theory as a guideline to develop an effective K-matrix interaction [83, 95, 77]. The K-matrix theory suggests that the interaction due to many body effects should depend on local density and on starting energies. The dependence on angular momentum can be expressed as a non-locality in the two-body interaction. It is in itself interesting to find out if such an interaction is capable of describing nuclear properties. Of an even larger value would this approach be if it turns out that such a microscopic model of the nucleus is manageable enough to compete with the sophisticated semi-empirical mass formula developed by Myers and Swiatecki [47].

This question is essential when one wishes to extend the many body calculations to deformed and superheavy nuclei. So far the most reliable calculations of this kind have been made using the mass formula, the Nilsson model and the Strutinsky corrections. In this, essentially macroscopic

theory, one is at each step of the calculations making sure that experimental data are reproduced accurately. In order for the purely microscopic many body theory to compete successfully with the macroscopic theory it is necessary to reproduce the known data equally well or even better because the microscopic theory is inherently more powerful. Shell effects, curvature corrections, etc. are built into the theory and do not have to be added on.

In the macroscopic model the parametrization consists of volume-, surface- and symmetry-energies etc. In the microscopic model the two-body interaction is parametrized. Although a parametrized microscopic theory has not been in the mind of all workers in this field we believe that it is the most logical and powerful interpretation of these type of calculations. This will make it directly competitive with the macroscopic model. It has been the philosophy behind the models developed in ref. [83]. The parameters of the Skyrme III force were evidently derived with the same purpose in mind. This force gives good agreement with bindings of nuclei through the periodic table [96].

Referring to ref. [83] it was there found that already a simple interaction, model A, can reproduce binding energies of closed shell nuclei. The interaction of model A is non-local represented by a quadratic momentum dependence, but independent of many-body effects. This model contained five adjustable parameters, one of which was used to adjust the spin–orbit splittings. The calculated single particle spectrum, removal energies, agreed however rather poorly with the known spectra around the Fermi surface. The simple model would therefore not reproduce binding energies of nuclei between closed shells.

An important conclusion that one can draw from the Brueckner theory is however that the K-matrix interaction depends on the nuclear medium. The simplest way to describe this would be by a density dependent force. This is done in the model C of ref. [83]. This model reproduces binding energies of closed shell nuclei and also the single particle spectrum of these nuclei with surprising accuracy. It is actually well recognized by workers in this field that a density dependence is required to get good agreement.

The density and momentum dependent interaction has of course some features similar to those of the interaction used by Brueckner et al. [53]. This was critized above on the grounds that the interaction should also depend on starting energies. The approaches are however quite different in the two investigations. Brueckner et al. calculate the K-matrix from a nucleon–nucleon force. The approach of ref. [83] is semiphenomenological and the question asked is whether a chosen model, by adjustments of its parameters is capable of describing the experimental data.

Based on our knowledge of the nucleon–nucleon force (which is far from conclusive however) a dependence on starting energies seems inevitable and it seems that a more realistic model should include these effects. It is of course included in Negele's work mentioned above. It is also included in the model D of ref. [83]. This model has been investigated further but it does not improve the results to include these effects [97]. This point has to be investigated further.

7. Single particle energies

We have already in previous sections seen that the concept of single particle energies plays an important role in the development of the many body theory. It is for example important in the definition of the K-matrix, eq. (3.11). We have further discussed the shell-model potential at

length. The eigenvalues of the shell-model Hamiltonian defines single-particle energies and these are not necessarily the same as those defining the K-matrix. This was discussed in sects. 5.1 and 5.4. Neither of these energies relate a priori to any experimental determination of such energies. It is, as a matter of fact, not even possible to define a unique or "universal" single particle energy.

It is on the contrary convenient, see e.g. ref. [77], although not always necessary (especially in certain approximations), to distinguish between the following single-particle energies:

i) ϵ_λ, the eigenenergies of the shell model potential U_{SM} defined in sect. 5,

ii) e_λ, the energies appearing in the definition of the K-matrix, sects. 5.1 and 5.4,

iii) S_λ, the "experimental" single particle energy.

We shall in this section primarily discuss the removal or separation energy, S_λ. We shall furthermore distinguish between $S_\lambda(\infty)$ and $S_\lambda(0)$, corresponding to slow and fast removals, $\Delta t = \infty$ and $\Delta t = 0$, respectively. To what extent such a distinction is physically motivated is not quite clear but the distinction can at least be made mathematically. In subsection 7.2 we shall separately discuss the concept of rearrangement energy, which plays an important role in Brueckner theory but which has been the subject of numerous misconceptions. We shall only briefly discuss *addition* energies.

Before dealing with the problem of removal energies for nuclei with strong two-body correlations, we feel that it is instructive to briefly review the similar problem in atomic physics neglecting two-body correlations. In the derivation of the Hartree–Fock potential by Rayleigh–Ritz variational method one introduces Lagrangian multipliers. These multipliers are mathematical entities and have *a priori* no physical meaning whatsoever. In the solution of the Hartree–Fock equations they formally appear like single particle energies but that does still not identify them with any experimental quantities. It was shown by Koopmans [98], however, that the multipliers are, to some approximation, equal to the removal energies. This follows quite simply from the fact that an observed energy of removal is equal to the energy of the atom minus the energy of the ion, the electron being removed out of some orbit. In order to derive this theorem of Koopmans' it is necessary to assume the approximation that the Hartree–Fock field of the ion is the same as that for the atom. Koopmans also considers corrections to his theorem and mentions explicitly "die Kontraktions Korrektion" (the contraction correction) resulting from the change in single particle orbitals, i.e. change in Hartree–Fock field, as (or after) an electron is removed. We shall refer to this correction as an *orbital rearrangement* correction or energy.

If one neglects the orbital rearrangement energy, i.e. applies Koopmans' theorem and thus compares the eigenvalues of the Hartree–Fock field of the atom with atomic spectra the agreement with experiment is to within about 10% [99]. One conveniently corrects for the orbital rearrangement energy by calculating the removal energy as the difference between the energy of the atom and that of the ion. The energy of the ion is now calculated with the Hartree–Fock field for the ion. If it were calculated with the Hartree–Fock field of the atom one would simply get Koopmans' theorem. The correction due to orbital rearrangement improves the agreement with experimental spectra to within about 2% [99].

These agreements of 10% and 2% respectively refer to energies of photons emitted subsequent to the creation of a hole. The conclusion as regards the physical processes involved is that the rearranged state is indeed a good approximation to the true eigenstate. Also the rearrangement process must have taken place before the decay, because otherwise this state would not show up as the predominant state.

There is another way of calculating the orbital rearrangement energy than the one described above. The linked cluster expansion is valid in any basis set. For a system of A particles all diagrams with bubble insertions are cancelled by the similar diagrams with potential insertions is the potential is defined by Hartree–Fock for the A particles. For example, the diagrams 1b and 1d are all cancelled (or included) if the potential is so defined. If one now removes a particle λ the Hartree–Fock field changes but one can still calculate the energy of the $A-1$ system using the basis set of the A particle Hartree–Fock potential.

Doing so one finds that the removal energy, i.e. the difference in energy between the A and the $A-1$ system is given by the diagrams in fig. 6. Diagram 6a is the Hartree–Fock energy while diagram 6b, with $\lambda = \lambda'$, is the main contribution to the orbital rearrangement energy. It involves a 1h-state coupled to 1h1p-states. (In the Hartree–Fock basis it is exactly these 1h1p-states that are minimized.) The admixing causes a shift of the λ-hole, equal to the orbital rearrangement energy but the hole-strength also gets dissolved into the 1h1p-states. It is trivial to show that the splitting is such that the *centroid* of these states is equal to the unperturbed Hartree–Fock energy. Thus

$$e_\lambda = \sum_i S_{i,\lambda}\, \epsilon_\lambda^{(i)}. \tag{7.1}$$

Here $S_{i,\lambda}$ is the strength function; it is the strength of hole-state λ in the perturbed state i. In a fast removal (see sect. 7.3) one expects to see all the levels $\epsilon_\lambda^{(i)}$ excited with the strengths $S_{i,\lambda}$. The centroid of these levels should therefore satisfy Koopmans' theorem. An analysis of this type has been made by Meldner and Perez [100]. In a slow removal (sect. 7.1) the orbits rearrange during the time of removal and only one level, the one with rearranged energy, carries all the strength. It can be calculated by either of the two methods described above. Customarily it is calculated by the first method finding the Hartree–Fock field for the ion.

7.1. Slow removals

Much of the discussion regarding electron-removals from atoms can be carried over to the problem of nucleon-removals from nuclei. The difference between the two problems result from the nucleon correlations. Removal energies are basically the difference in energy between two systems. For atoms these energies are adequately calculated by Hartree–Fock theory. For nuclei the energies are well approximated by an application of Brueckner theory. We shall find that the result of the strong correlations lead to interesting and important effects as regards the removal energies.

In this subsection we shall discuss slow removals. Experimentally well defined and well known for most nuclei is the removal or separation energy

$$-S(\infty) = E_A - E_{A-1} \tag{7.2}$$

where $S(\infty)$ indicates that the nucleon is removed adiabatically so that each of the systems A and $A-1$ are in its respective ground state. Less well-defined is the removal energy

$$-S_\lambda(\infty) = E_A - E_{A-1}^\lambda \tag{7.3}$$

referring to the removal of a nucleon from single-particle state λ. This first of all requires a definition of state λ which explicitly refers to a shell-model orbital yet to be defined both experimentally and theoretically. Furthermore, E^{λ}_{A-1} refers to an excited state, which necessarily will decay, thus contradicting the statement that the removal is adiabatic. However, if an orbital λ is defined one can calculate the energy E^{λ}_{A-1} of the nucleus $A-1$ in this hole-state configuration. One can also calculate the decay time or width of this excited hole-state. The slow removal has thus to be made faster than this decay time in order for this definition to be meaningful. For atomic spectra there is experimental evidence that the corresponding definition is meaningful, as discussed in the introduction to this section.

Calculating the energies in eq. (7.3) by the K-matrix approximation (3.10) for the energy in some (fixed) basis set one finds the diagrammatic expansion for the removal energy $S_{\lambda}(\infty)$ to be given in fig. 6. This seems identical to the expansion for the electron (uncorrelated) removal energy. There is however important differences. First diagram 6b now also includes states $\lambda' \neq \lambda$ and more important, all interactions are K-matrix interactions. The second order diagram, 6b, with $\lambda' \neq \lambda$ was referred earlier to as an orbital rearrangement term. This does not contribute in infinite nuclear matter and all three higher order diagrams in fig. 6 are usually referred to as *Brueckner rearrangement* energies. They were first calculated by Brueckner and coworkers [43] but rearrangements were first discussed in a much earlier paper of Brueckner [31] in relation to his theory. The rearrangement effect plays an important role in understanding the nuclear many-body theory and we therefore devote the next subsection to this subject. We also bring up some of the historical developments in relation to rearrangement.

7.2. Rearrangement energies

The terminology as regards "rearrangement energy" has come to be somewhat diversified in the literature on nuclear many body theory. It has often been of a different meaning to different authors. The word "rearrangement" itself implies a change of some sort of the nuclear structure and this was also its original meaning.

Thus, Koopmans may have been the first to refer to the orbital rearrangement energy, and this is a rearrangement effect in the true sense.

The Brueckner theory is a treatment of nuclear correlations. These correlations depend on the presence of other nucleons. This is seen explicitly in the K-matrix equation (3.11). It is therefore to be anticipated that the correlation structure changes upon removal, or excitation of a nucleon. Brueckner discusses this in some detail in one of his earlier papers and points out that the change in structure, or rearrangement, should play an important role in our understanding of the nuclear single particle structure [31].

We have emphasized earlier that single particle energies play an important role in the definition of the K-matrix in eq. (3.11). We discussed in sects. 4 and 5 that by a proper choice of single particle energies, when defining the K-matrix, one can achieve a summation of important diagrams. There is (as also pointed out in the beginning of sect. 7) no *a priori* reason to expect that the single particle energies so chosen have any physical meaning. Nevertheless some of Brueckner's work [22] was criticized for its failure to satisfy a relation between separation energy $S(\infty)$ and binding energy for an infinite system [101]. The relation we refer to is the so-called Hugenholtz–van Hove theorem [101] which states that for an infinite system

$$-S(\infty) = E/A + p/\rho \tag{7.4}$$

where ρ is the density and p is the pressure

$$p = -(\partial E/\partial V)_A = \rho^2 \frac{\mathrm{d}}{\mathrm{d}\rho}(E/A) . \tag{7.5}$$

At saturation $p = 0$ and

$$E_F = -S(\infty) = E/A \tag{7.6}$$

where E_F is the single particle energy at the Fermi momentum. The relation (7.6) also follows directly from eq. (7.2) and the fact that E is an extensive thermodynamic function, i.e.

$$E_A = A \cdot (E/A) . \tag{7.7}$$

Hugenholtz and van Hove [101] criticized the calculations of Brueckner and Gammel [22] for the reason that the single-particle energies and total energy of ref. [22] did not satisfy eq. (7.6). They concluded that important contributions to E_F or to E or both were neglected in Brueckner theory. The reason for the discrepancy is now well understood and the criticism was really unjustified. Brueckner's theory was originally designed to calculate the total energy of the system. To do so single-particle energies had to be defined for the purpose of defining the K-matrix by eq. (3.11), but as pointed out above, these energies e_λ bear no direct relation to any experimental definition. However, once the total energy is well approximated the single particle energy $E_F = S(\infty)$ can be found from eq. (7.2). One then finds that e_F and E_F differ exactly by the Brueckner rearrangement terms first mentioned at the end of sect. 7.3. Brueckner [102] actually also showed that the relation (7.6) is easily re-established just by redefining all the single particle energies e_λ by adding a constant term. This will not change the definition of K. One would thus simply put $e_\lambda \to e_\lambda + \Delta$ with Δ determined from $e_F + \Delta = E_F$. Hugenholtz and van Hove also criticize this procedure on the grounds that the e_λ are strongly momentum dependent and that there is no basic reason why the Δ should be constant. One must, however, realize that the Δ like the e_λ are purely mathematical quantities. It is on the contrary convenient to separately define S_λ and e_λ as indicated in the beginning of sect. 7.

Brueckner, Gammel and Kubis [43] calculated the higher order contributions to $S_\lambda(\infty)$ given by the diagrams in fig. 6. They found that the relation (7.6) was then well satisfied with E calculated from eq. (3.10).

They also considered corrections to E by putting insertions in hole-lines but concluded those corrections to be small. This is discussed in sect. 4.

The Brueckner rearrangement energies relate to changes in the two-body correlations in the residual nucleus when a nucleon is removed. The second order, fig. 6b, results from Q_A being different from Q^λ_{A-1} in the K-matrices (3.11) used to calculate S_λ from eq. (7.1). The third orders, figs. 6c, d, result from the change in the energy denominator of the K-matrix (3.11) as a nucleon is removed. All these diagrams have been calculated [43, 44, 55, 70, 71, 103]. The diagram 6c is related to 6a by eq. (4.3). Consequently these two diagrams have the same momentum dependence or nonlocality. The second order rearrangement energy is complex. It involves energy conserving transitions corresponding to the decay of the $A-1$ system. Both the real and imaginary parts are strongly momentum dependent. In nuclear matter the real part is 25 and 5 MeV approximately at

the bottom and surface of the Fermi sea respectively. The third order diagram gets most of its contributions from the short ranged and tensor parts of the interaction while the second order is mostly due to the long ranged central part, except at the Fermi surface where the tensor component is the important contribution.

Considerable attention was given to the concept of rearrangement energy following Hugenholtz and van Hove's criticism. We mention as examples the works of Thouless [104], Brenig [105] and Mittelstaedt [106].

As mentioned earlier the original reason for the choice of the word "rearrangement" is that it refers to a change in structure of the nucleus. Through the work of Hugenholtz and van Hove the attention was focused on the difference between Brueckner's e_F and the removal energy S_F. The K-matrix energies e_λ are in many formulations of the Brueckner theory following Goldstone [7] referred to as model energies. Some authors have therefore adopted a terminology in which they refer to it as a "rearrangement energy" the difference between the single particle energy of their specific model and the removal energy. This is really a misuse of the concept of rearrangement and leads to misleading statements.

The third-order diagram in fig. 6 is usually called a rearrangement diagram. The origin of this terminology is that K is changed as a result of the change in the energy-denominator when a particle is removed (or added). But this is a somewhat arbitrary observation. This method of generating the third-order diagram is a result of a definition rather than a physical consequence. The two body K-matrix is defined by the choice of e_λ so that the diagrams 8a and 8c are included in the total energy and diagrams 6c and 6d are then generated upon removal. Diagrams 8a and 8c are however basically three-body diagrams and can be regarded as corrections due to interaction of the bubble nucleon with a correlated pair rather than an uncorrelated nucleon as in diagram 1a. This latter interpretation is probably the physically correct one as the result presented in the next subsection will show.

Orbital rearrangement energies have also been calculated for nuclei but are found to be relatively smaller than the Brueckner rearrangement [107, 108].

7.3. Fast removals

The distinction between fast and slow removals of nucleons is mainly theoretical. To what extent this is experimentally justified is far from clear, other than in the very extreme case as discussed in subsection 7.1 on slow removals. Usually one refers to the knock out, (e, e'p) and (p, 2p) experiments as examples of fast removals. They are therefore examples of reactions where the impulse approximation should be valid. The review articles by Jacob and Maris refer especially to these reactions [109]. Deeper shells have also recently been studied with the (p,d) reactions [110].

These experiments give information on the deeper shells in light nuclei, and are actually the only such experiments that give any indication that a shell-model description of these deeper states at all make sense. We shall now proceed to present a short analysis of the single particle energies obtained from these experiments.

In atomic physics one can test Koopmans' theorem [100] and to some extent the orbital rearrangement correction directly from experiments as described in the beginning of this section. For nuclei a similar test is not possible simply because the nucleon force is not known accurately enough. One can however make a somewhat similar test by a consistency investigation. In

Hartree–Fock (first order uncorrelated theory) one has

$$E = \tfrac{1}{2} \sum_{i<A} (\eta_i + t_i) \tag{7.8}$$

where E is the total binding energy of the system of A particles, η_i is the Hartree–Fock potential single particle energies and t_i the kinetic energies. From eq. (3.10) one finds that eq. (7.8) is valid also in Brueckner theory whence η_i is the K-matrix single particle energy, in eq. (3.11) denoted by e_i. This can be rewritten somewhat by putting

$$e_i = \eta_i + e_i^{\mathrm{r}} \tag{7.9}$$

where e_i now are the removal energies and e_i^{r} the rearrangement energies. In atomic Hartree–Fock it would be the orbital rearrangement energies. Then eq. (7.8) can be written

$$E = \tfrac{1}{2} \sum_{i<a} (e_i + t_i) - \tfrac{1}{2} \sum_{i<A} e_i^{\mathrm{r}}. \tag{7.10}$$

The total energies E are well known. The kinetic energies t_i are slightly model-dependent but are essentially determined by the well known nuclear radii. Taking the experimental energies e_i from the knock out experiments the last sum or the average e_i^{r} can be calculated. This was done by Köhler [103] and repeated by Elton [111] and Becker [112] who also made a correction for center of mass motion. The results are summarized in table 2. Although the results differ somewhat essentially because of the use of different experimental knock out data they all agree that an average 6–8 MeV rearrangement energy is necessary to satisfy the experimental data. This correction is too large to be explained by orbital rearrangement [107, 108], but is perfectly understandable in view of the calculated Brueckner rearrangements discussed earlier. This test of eq. (7.10) is therefore as direct a test as one can do of the applicability of Brueckner theory for nuclear correlations.

There is still, however, some question as to how to interpret the results of this analysis. If it were the question of slow removals our discussion in subsection 7.1 showed that we should expect to find that rearrangement energies would contribute to the single particle energies. But here we are dealing with fast removals.

It has in fact been argued that for fast removals rearrangements would not contribute as the nucleus would then not have time to rearrange before the knock-out [113]. If this were the case, which physically indeed seems very reasonable, one would expect the analysis of the knock-out data described above not to result in any rearrangement energies at all. The situation has evidently to be clarified.

It should first of all be observed that the energies of the removal spectrum are not determined by the speed of the removal but they refer only to the energy difference between the initial and final nucleus. The former nucleus (of A nucleons) is in its ground state and the latter ends up in some state being an eigenstate of the $A-1$ nucleon system. In the case of deep removals these would be highly excited states that would be expected to be of a complex structure. In the corresponding case of atomic physics they are mainly pure hole-states but cannot be expected to be so for the strongly interacting nuclear system.

Table 2
Rearrangement energies in MeV calculated by eq. (7.10) from experimental binding energies and single particle energies.

	^{12}C	^{16}O	^{28}Si	^{32}S	^{40}Ca	^{56}Ni
Köhler [103]	11	8	3.7(^{27}Al)			
Elton [111]	6.1	4.2	1.6	1.8	5.4	
Becker [112]	6–7	6.1–6.8	12.8	13.2	8.0	8.2

It is evident that a more detailed understanding is required of the spectrum of states resulting from the fast removal. For this purpose it is convenient to define the spectral function $P(\lambda, E)$ which is the strength of state λ to be found at energy E. Here λ denotes all shell-model quantum numbers nl_j. Experimentally one can usually determine l and j but the radial quantum number n is undetermined or has to be more or less guessed. Some detailed discussion of the experimental information on the spectral function can be found in a recent review article by Hodgson [114].

We shall now assume that the knock-out reaction can be described by the impulse-approximation [109] which is consistent with the idea of a fast removal. Then the theoretical expression for the spectral function will be [115]

$$P(\lambda, E) = \langle A|a_\lambda^+ \delta(E-H)a_\lambda|A\rangle = \sum_f |\langle f|a_\lambda|A\rangle|^2 \delta(E-E_f) \tag{7.11}$$

where a^+ and a are creation and annihilation operators. E_f is the energy of final state of the $A-1$ system.

Once this is established several useful results can easily be derived. So for instance, the centroid energy is

$$E_\lambda = \int_{-\infty}^{+\infty} EP(\lambda, E)\,dE \Big/ \int_{-\infty}^{+\infty} P(\lambda, E)\,dE\,. \tag{7.12}$$

The nominator is the ground state expectation value of the operator

$$H_\lambda = a_\lambda^+ [a_\lambda, H] \tag{7.13}$$

while the denominator is the ground state value of the number operator

$$N_\lambda = a_\lambda^+ a_\lambda\,. \tag{7.14}$$

Koltun [115] has given the linked cluster expansions of these operators and concludes that diagram 6b does not contribute to the centroid energy (7.12) while the rest of the diagrams 6 do He does not consider diagram 6d which is probably small anyway.

This important result agrees with the results obtained in the Green function formalism [116, 117]. This result concerning the centroid energy is not trivial to apply to the experimental spectral function because it involves integrations over all energies for each state λ. It does however immediately shed some light on the results of the analysis above on the basis of eq. (7.10). The intuitive result discussed above concerning the contribution of rearrangement energies turned out to be wrong. The third order rearrangement energies 6c and 6d contribute to the centroid

energy. If one therefore inserts in eq. (7.10) the experimentally measured centroid energies for e_i the average rearrangement energy thus determined should refer to the third order rearrangement energies. Becker [112] assumed that these were indeed the rearrangement energies that he determined and found this to be in numerical agreement with other estimates of these energies.

The energies e_i that were used in eq. (7.10) were at the maxima of the spectral function. There is large uncertainty whether these are also the location of the centroid. It is probably true for the deepest states but not for states close to the Fermi surface.

To arrive at this conclusion requires a discussion of the second order diagram 6b. While diagrams 6c and 6d shift the whole strength of the levels the diagram 6b splits the strength of the levels into components, as seen explicitly in the calculations of Becker [118] and of Lipperheide et al. [119] for finite nuclei. In addition to this spreading width there is also a decay width. This decay width results from diagram 6b when the energies satisfy

$$e_\lambda + e_a = e_{\lambda'} + e_\alpha . \tag{7.15}$$

For this to occur a has to be a continuum state. This can always occur for an infinite medium but for a finite system it requires

$$e_\lambda \leqslant 2e_F \tag{7.16}$$

where e_F is the Fermi energy. Thus it does not occur for the states λ at the Fermi surface. The decay mechanism described by diagram 6b is in atomic physics referred to as the Auger effect. It has been calculated by diagram 6b for the neon atom [120]. The width has also been calculated for 1s-states for some finite nuclei and shown in table 3 [103]. The agreement with experiment is remarkably good.

The deep states are coupled to many other states, many of them are in the continuum. The unperturbed λ-state is therefore largely depleted and the broad peaks seen corresponding to deep removals are the many 2h1p states and the maximum is the centroid energy. The states close to the Fermi surface is coupled to states relatively further away. The depletion is less and the peaks seen are the shifted hole-states. The centroid energy lies deeper down and is not readily available. This is also the conclusion of Dieperink and Brussaard who estimate that the spreading width of states near the Fermi surface should be larger than observed [121].

This interpretation of the experimental evidence is probably correct, although more theoretical analysis would be desirable. A more detailed experimental analysis does unfortunately not appear feasible at least at present.

The conclusion that we like to draw from the above discussion is that in the fast removal experiments the deeper maxima show the location of the centroid energies, while the higher lying states show up as maxima shifted by the second order diagram. It is therefore required that a calculation of this diagram is made before comparison with experimental single particle energies for the states around the Fermi surface. Such a calculation has recently been made by Padjen et al. for ^{16}O [122]. It has been included in an approximate way in calculations on ^{208}Pb and other nuclei [83].

We like to return briefly to the finding of Koltun and others that the third-order diagrams contribute to the centroid energy of a fast removal. This may seem contradictory to our intuitive feeling that rearrangement energies would not contribute to a fast removal. The ad hoc reasoning behind naming the third order diagram a rearrangement energy was mentioned at the end of

Table 3
Calculated [103] and experimental widths of 1s-states in MeV.

	^{8}Be	^{12}C	^{16}O	^{27}Al	^{40}Ca	^{208}Pb
Calc.	8.1	11.5	13.7	19.6	21.6	29.8
Exp.	10(^{9}Be)	9–13	14	20	~20	

sect. 7.2. The result of Koltun and others substantiates the suggestion made there not to refer to these diagrams as rearrangement energy diagrams.

We have here discussed only fast removals but have so far neglected discussing fast *additions*. It was shown by Baranger that if additions as well as removals are included in the definition of the centroid energy in eq. (7.12) then all diagrams connected by a v-interaction to the hole line contribute [79]. For the fast removal it is rather all K-interaction diagrams that contribute. The physical explanation of the difference lies in the fact that the fast addition of a nucleon requires this nucleon to correlate with the other nucleons. This implies that for a high energy stripping reaction very high energies would be excited. The consequences of this appear not to have been investigated.

Koltun has brought to the attention an important sum-rule that is well-known in solid state physics. It relates the total energy E_A of a system to the spectral functions by [123]

$$E_A = \tfrac{1}{2}\int \mathrm{d}E \int \mathrm{d}k \left(\frac{k^2}{2m} - E\right) P(k,E)\,. \tag{7.17}$$

It is important that this relation, here given for an infinite system, is valid only if the total Hamiltonian includes one and two-body terms. It is also important to note that the E-integration goes over *all* energies. It is therefore not equivalent to eq. (7.8) or eq. (7.10) where the summation goes over occupied states only. The two expressions for the total energy is therefore compatible if we also remember that the centroid energy includes the third-order rearrangement energy while the η's in eq. (7.8) include K-matrix energies to first order only.

Koltun subjected eq. (7.17) to experimental test using (p,2p) data and found satisfactory agreement [123]. Recent results of Bernheim et al. do however not give that good agreement [124]. They analyzed their ^{12}C(e, e'p) data and found a binding energy per proton of -4.0 ± 0.5 MeV while the experimental binding energy per proton is -6.93 MeV. In principle any discrepancy would be attributable to three-body forces in the Hamiltonian. The experimental limitation on the high-energy tail of $P(k,E)$ in eq. (7.17) gives however another source of error. This correction was considered in the latest paper of ref. [119] and was then found to add another 1.7 MeV to the binding. Another physically important effect that would cause a discrepancy would be if the removals were indeed not fast in the sense that is assumed theoretically. Then one should expect some shift of the strength due to the second order rearrangement energy.

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