MASTER

The Ground State of Homogeneous Nuclear Matter
and the Foundation of the Nuclear Shell Model

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I. Introduction

Quantum theories of many-body systems fall into two broad classes: those that attempt to find the eigenfunctions of the Hamiltonian, and those that set up equations for bilinear functionals of exact eigenfunctions—that is, density matrices or Greens functions.

These lectures will be concerned only with the former approach. More specifically, we assume that there is an unperturbed reference state Φ and all other states under consideration are represented by

$$\Psi = \Phi + \Psi' , \quad (I.1)$$

where

$$(\Psi', \Phi) = 0 . \quad (I.2)$$

The state Φ will be a single Slater determinant describing a closed-shell nucleus or the normal state of noninteracting Fermi gas.

If a state Ψ represented as in Eq. (I.1) is an eigenstate of the Hamiltonian H , then the energy E is given by

$$E = (\Phi, H\Psi) . \quad (I.3)$$

For other nearby vectors Ψ the expression $(\Phi, H\Psi)$ need not be larger than the lowest eigenvalue. There will be no variational principle.¹

The main emphasis will be mathematical. The purpose is to set up equations for well-defined mathematical quantities such

¹By variational principle I understand a statement that a certain functional has an extremum.

that there is a definite existence problem for the solution and existence theorems can be proved.

In practice all we can obtain at best are approximations to the solution. In this connection I would like to emphasize the distinction between two kinds of approximations, namely between the approximation of the real world by suitable theoretical models and approximations to the solution of a mathematically well-defined problem. Once the Hamiltonian has been fully specified, we are concerned only with the latter. For mathematical approximations, we need a precise quantitative definition of neighborhood. What do we mean if we say a function is near the solution to the problem, or two solutions are near each other?

States may be represented by the set of correlated pair-excitation amplitudes. These amplitudes are square-integrable functions for finite systems. For qualitative considerations it is most convenient to think of very large systems as finite and to keep track of the volume dependence of different expressions. But for numerical calculations it is necessary to approximate very large finite systems by infinite systems—not the other way around. It is therefore more convenient to deal from the beginning with mathematical entities that are well defined for the translationally invariant system of infinite volume. If Φ is the translationally invariant normal state of a noninteracting Fermi gas, there can be no other translationally invariant state that is not orthogonal to Φ .² But the correlated pair-excitation amplitudes exist as translationally invariant generalized functions. A suitable topology for them is suggested by an examination of the density matrix

$$\langle x' | \rho | x \rangle = (\Psi, c^+(x) c(x') \Psi) / (\Psi, \Psi), \quad (\text{I. 4})$$

²R. Haag, Kgl. Danske Videnskab. Selskab, Mat.-Fys. Medd 29, No. 12 (1955). See p. 31.

where $c(x)$, $c^+(x')$ are nucleon annihilation and creation operators satisfying the commutation rules³

$$\{c(x), c^+(x')\} = \delta(x - x') . \quad (I.5)$$

The right-hand side of Eq. (I.4) should exist even for homogeneous systems, for which the numerator and denominator do not exist separately. Approximations are based on the idea that the correlated pair-excitation amplitudes are small except when the relative distances between particles are much less than their average distance.

The Schrödinger equation implies a set of nonlinear equations for the pair-excitation amplitudes. As a mathematical structure, these equations ask for a fixed point of a nonlinear mapping of a Banach space⁴ into itself.

For soft potentials the Hartree-Fock approximation is a suitable starting point, and corrections are obtained systematically by expansion in powers of the potential. For hard potentials the Brueckner approximation and systematic corrections arise naturally from qualitative assumptions about the pair-excitation amplitudes. The first corrections to the Brueckner approximation are identical with Bethe's three-body corrections.⁵ Formally, the approximations are an expansion in powers of density.

These developments have implications for the ground-state problem of closed-shell nuclei as well as the shell-model problem. They will be sketched in sections VI and VII.

³ Spin and isospin indices are suppressed from the notation for convenience.

⁴ A Banach space is a complete linear space for which a distance (norm) is defined.

⁵ See R. Rajaraman and H. A. Bethe, Rev. Mod. Phys. 39, 745 (1967) and references quoted there.

II. States of Low-Density Fermion Systems

This section presents the mathematical machinery used in the representation of states.⁶ The states may or may not be stationary; dynamical considerations are postponed to the next section. The Hamiltonian and its properties are, at the moment, irrelevant.

The state Φ is represented by a single Slater determinant containing the orthonormal function $\varphi_\nu(x)$, $\nu = 1, \dots, N$. The single-particle projection operator Λ is defined by

$$(x' | \Lambda | x) = \sum_{\nu=1}^N \varphi_\nu(x') \varphi_\nu(x) . \quad (\text{II. 1})$$

The particle-destruction operator $a(x)$ and hole-destruction operator $b(x)$ are defined by

$$a(x) = \int dx' (x | 1 - \Lambda | x') c(x') , \quad (\text{II. 2})$$

$$b(x) = \int dx' c^\dagger(x') (x' | \Lambda | x) . \quad (\text{II. 3})$$

The state Φ satisfies the equation

$$d(x) \Phi = 0 , \quad (\text{II. 4})$$

where

$$d(x) \equiv a(x) + b(x) . \quad (\text{II. 5})$$

Equation (II.4) determines the state Φ uniquely.

⁶F. Coester, Nucl. Phys. 7, 421 (1958); F. Coester and H. Kümmel, Nucl. Phys. 18, 888 (1960).

Any state vector Ψ that is not orthogonal to Φ and is normalized by

$$(\Phi, \Psi) = 1 \quad (II. 6)$$

may be represented in the form

$$\Psi = F \Phi, \quad (II. 7)$$

where

$$F = 1 + \sum_{n \geq 1} F_n \quad (II. 8)$$

and

$$F_n = \frac{1}{(n!)^2} \int dx_1 \cdots \int dx_n \int dy_1 \cdots \int dy_n a^+(x_1) \cdots a^+(x_n) b^+(y_n) \cdots b^+(y_1) \\ \times F_n(x_n, \cdots, x_1; y_1, \cdots, y_n). \quad (II. 9)$$

The amplitudes F_n must be square integrable since

$$\|\Psi\|^2 = (\Psi, \Psi) = 1 + \sum_n \frac{1}{(n!)^2} \int dx_1 \cdots \int dx_n \\ \times \int dy_n \cdots \int dy_1 |F_n(x_1, \cdots, x_n; y_n, \cdots, y_1)|^2. \quad (II. 10)$$

They are the probability amplitudes for the presence of n particle-hole pairs. It is convenient and always possible to define an operator S .

with the same formal structure,

$$\underline{S} = \sum_{n \geq 1} \underline{S}_n, \quad (\text{II.11})$$

$$\underline{S}_n = \frac{1}{(n!)^2} \int dx_1 \cdots \int dx_n \int dy_n \cdots \int dy_1 a^+(x_1) \cdots a^+(x_n) b^+(y_n) \cdots b^+(y_1)$$

$$\times \underline{S}_n(x_n, \cdots, x_1; y_1, \cdots, y_n),$$

such that

$$\underline{F} = e^{\underline{S}}, \quad (\text{II.12})$$

since the equations

$$\begin{aligned} \underline{F}_1 &= \underline{S}_1 \\ \underline{F}_2 &= \underline{S}_2 + \frac{1}{2} \underline{S}_1^2 \\ \underline{F}_3 &= \underline{S}_3 + \underline{S}_1 \underline{S}_2 + \frac{1}{3!} \underline{S}_1^3 \\ &\dots \end{aligned} \quad (\text{II.13})$$

can always be solved to give

$$\begin{aligned} \underline{S}_1 &= \underline{F}_1 \\ \underline{S}_2 &= \underline{F}_2 - \frac{1}{2} \underline{F}_1^2 \\ \underline{S}_3 &= \underline{F}_3 - \underline{F}_1 \underline{F}_2 + \frac{1}{3} \underline{F}_1^3 \\ &\dots \end{aligned} \quad (\text{II.14})$$

The form (II.12) for F is convenient because the inverse of $e^{\underline{S}}$ has the form $e^{-\underline{S}}$. We shall see that the transition to infinite homogeneous systems can be made most easily for the amplitudes S_n .

It is readily apparent from Eq. (II.10) that the amplitudes F_n cannot be square integrable if they are invariant under translations. States of a homogeneous system are described by translationally invariant amplitudes F_n that are in some sense limits of square integrable functions. A discussion of the single-particle density matrix provides heuristic considerations that will make this limit precise.

The unperturbed density matrix is

$$(x' | \rho_0 | x) = (\Phi, c^+(x) c(x') \Phi) = (x' | \Lambda | x) . \quad (\text{II. 15})$$

We want to impose conditions on Ψ such that the perturbed density matrix (I.4) differs from ρ_0 only by small corrections. From

$$\Psi = e^{\underline{S}} \Phi , \quad (\text{II. 16})$$

it follows that

$$d(x) \Psi = [d(x), \underline{S}] \Psi . \quad (\text{II. 17})$$

From (I.4) and (II.17), it follows that

$$\begin{aligned} (x' | \rho - \rho_0 | x) = & (\Psi, [a^+(x) b^+(x') + b(x) a(x') + a^+(x) a(x') \\ & - b^+(x') b(x)] \Psi) / (\Psi, \Psi) \end{aligned}$$

$$\begin{aligned}
&= (\Psi, \left[\{b(x'), [a(x), S]\}^+ + \{b(x), [a(x'), S]\} \right. \\
&+ [b(x'), S]^+ [a(x), S]^+ + [b(x), S] [a(x'), S] \\
&\left. + [a(x), S]^+ [a(x'), S] - [b(x'), S]^+ [b(x), S] \right] \Psi) / (\Psi, \Psi).
\end{aligned} \tag{II. 18}$$

The conditions for this to be small are simpler than one might expect.

Since the operators $[d(x), S]$ and F commute, we have

$$\begin{aligned}
\| [d(x), S] \Psi \| / \| \Psi \| &= \| F [d(x), S] \Phi \| / \| F \Phi \| \\
&\leq (\| F \| / \| F \Phi \|) \| [d(x), S] \Phi \|
\end{aligned} \tag{II. 19}$$

where $\| F \|$ is the operator norm of F defined by

$$\| F \| = \sup_{\Psi} \| F \Psi \| / \| \Psi \| \tag{II. 20}$$

We require therefore that the expressions $\| [d(x), S] \Phi \|$ and $\| \{b(x), [d(x), S]\} \Phi \|$ shall be sufficiently small, i.e., that

$$\frac{1}{\rho_0} \| [d(x), S] \Phi \|^2 \ll 1 \tag{II. 21}$$

and

$$\frac{1}{\rho_0} \| \{b(x'), [a(x), S]\} \Phi \| \ll 1 \tag{II. 22}$$

The condition (II. 21) and (II. 22) are compatible with translational invariance for S . If Eq. (II. 21) is satisfied for large finite systems, then the expression $\| S \Phi \|^2$ will be proportional to the volume.

Condition (II.21) suggests that a suitable norm for the operator S is

$$\|S\| = \sup_x \| [d(x), S] \Phi \| \quad (\text{II.23})$$

Completion under that norm defines a Banach space that contains translationally invariant elements. These translationally invariant elements are square-integrable functions of the relative coordinates. As such they form a Hilbert space.

The Fourier transforms $S_n(k_1, \dots, k_n, p_n, \dots, p_1)$ of these amplitudes are proportional to a δ function⁷

$$S_n(k_1, \dots, k_n, p_n, \dots, p_1) \quad (\text{II.24})$$

$$= \delta(k_1 + \dots + k_n - p_n - \dots - p_1) s_n(k_1, \dots, k_n, p_n, \dots, p_1),$$

where s_n is a square-integrable function over a $(6n - 3)$ -dimensional momentum space. All k 's are above the Fermi level and all p 's are below. Obviously $S_1 = 0$ since $\delta(k - p) = 0$.

Notice that the pair-excitation amplitude $S_2(x_1, x_2; p_2, p_1)$ is the correlated part $\zeta(r)$ of the two-body wave function of the many-body system and

$$\frac{1}{\rho_0} \|S_2\|^2 = \rho_0 \int d\tau |\zeta(r)|^2.$$

The norm $\|S_2\|$ is thus related to the familiar "volume of the wound" of the Brueckner theory.⁸

⁷ We shall generally use the convention that $f(k)$ or $f(p)$ is the Fourier transform of $f(x)$ for any function.

⁸ B. H. Brandow, Phys. Rev. 152, 863 (1966).

The condition (II.21) suggests an algorithm for the systematic expansion of density matrices.⁹ The convergence of that algorithm needs further investigation, which is left as a problem for the reader.

Problem: Let A be an operator that is a polynomial in the creation and annihilation operators. The operator A_c is defined as that part of A that contains after normal ordering at least one creation operator and no annihilation operators. Define a sequence of operators A_m by

$$A_1 = (e^{-S} A e^S)_c \quad (II.25)$$

$$A_m = (e^{-S} A_{m-1}^+ e^S)_c$$

and the numbers $\bar{A}_m$ by

$$\bar{A}_1 = \langle e^{-S} A e^S \rangle_0 \quad (II.26)$$

$$\bar{A}_m = \langle e^{-S} A_{m-1}^+ e^S \rangle_0 .$$

(1) Verify that the expectation value $\langle A \rangle \equiv (\Psi, A\Psi)/(\Psi, \Psi)$ is given by the identity

$$\langle A \rangle = \sum_{m=1}^N \bar{A}_m + \begin{cases} \langle A_N \rangle & \text{for odd } N, \\ \langle A_N^+ \rangle & \text{for even } N. \end{cases} \quad (II.27)$$

(2) For $A = c^+(x_1) \cdots c^+(x_n) c(x_n) \cdots c(x_1)$, derive necessary and sufficient conditions on S for the convergence of the limit $N \rightarrow \infty$.

⁹ The same techniques are also applicable to multiparticle density matrices, as shown in Ref. 6.

III. Stationary States of Homogeneous Nuclear Matter

For a homogeneous system, the particle- and hole-annihilation operators are defined by

$$a(\mathbf{x}) = (2\pi)^{-\frac{3}{2}} \int d\mathbf{k} c(\mathbf{k}) e^{i\mathbf{k} \cdot \mathbf{x}}, \quad (III.1)$$

$$|\mathbf{k}| \geq k_F$$

and

$$b(\mathbf{x}) = (2\pi)^{-\frac{3}{2}} \int d\mathbf{p} c^\dagger(\mathbf{p}) e^{i\mathbf{p} \cdot \mathbf{x}}, \quad (III.2)$$

$$|\mathbf{p}| \leq k_F$$

where $c(\mathbf{k})$ is the Fourier transform of $c(\mathbf{x})$. It is understood that for any single-particle momentum $|\mathbf{k}| \geq k_F$ and $|\mathbf{p}| \leq k_F$.

The constant particle density ρ_0 is

$$\rho_0 = \text{Trace}_{\sigma, \tau} (\mathbf{x} | \Lambda | \mathbf{x}) = \frac{4}{(2\pi)^3} \frac{4\pi}{3} k_F^3. \quad (III.3)$$

The trace is taken over spin and isospin variables σ, τ .

The Hamiltonian $\underline{H} = \underline{H}_0 + \underline{V}$ will be written as a space integral over a Hamiltonian density $\underline{H}(\mathbf{x}) = \underline{H}_0(\mathbf{x}) + \underline{V}(\mathbf{x})$, where

$$\underline{H}_0(\mathbf{x}) = c^\dagger(\mathbf{x}) (-\nabla^2/2m) c(\mathbf{x}) \quad (III.4)$$

and

$$\underline{V}(\mathbf{x}) = \frac{1}{4} \int d\mathbf{x}_1' \int d\mathbf{x}_2' \int d\mathbf{x}_1 \int d\mathbf{x}_2 \delta(\mathbf{x} - \mathbf{x}') \quad (III.5)$$

$$\times c^\dagger(\mathbf{x}_2') c^\dagger(\mathbf{x}_1') (\mathbf{x}_1' \mathbf{x}_2' | V | \mathbf{x}_2 \mathbf{x}_1) c(\mathbf{x}_1) c(\mathbf{x}_2),$$

with

$$(x_1' x_2' | V | x_2 x_1) = \delta(X' - X) (r' | V | r) , \quad (III.6)$$

$$X \equiv \frac{1}{2} (x_1 + x_2), \quad r \equiv x_1 - x_2 .$$

In a large box the normal state Φ of a noninteracting Fermi gas is an eigenstate of the Hamiltonian, and the eigenvalue is proportional to the volume. It is possible and convenient to avoid any reference to the volume of infinite systems. The normal state Φ of an infinite system is not in the domain of H_0 but it is well defined by

$$d(x) \Phi = 0 \quad (III.7)$$

and it is stationary, that is

$$[H_0, d(x)] \Phi = 0 . \quad (III.8)$$

The energy per particle is obtained from the Hamiltonian density $H_0(x)$ by

$$\varepsilon_0 = \frac{1}{\rho_0} (\Phi, H_0(x) \Phi) = \frac{3}{5} \frac{k_F^2}{2m} . \quad (III.9)$$

In the presence of interactions, we consider the functional

$$\Psi = e^S \Phi \quad (III.10)$$

and require it to be stationary. The state Ψ is stationary if

$$(H, \{d(x) - [d(x), S]\}) \Psi = 0 \quad (III.11)$$

or, equivalently,

$$[(e^{-S} H e^S), d(x)] \Phi = 0 \quad (III.12)$$

Equation (III.11) is satisfied if and only if the creation part of the operator $e^{-S} H e^S$ vanishes, i.e., if

$$(e^{-S} H e^S)_c \equiv [H_0, S] + (e^{-S} V e^S)_c = 0 \quad (III.13)$$

The subscript c denotes the pure pair-creation part of a normal ordered operator. Equation (III.13) is the equation to be solved.

The energy per particle is given by

$$\varepsilon = \frac{1}{\rho_0} (\Phi, e^{-S} H(x) e^S \Phi) \quad (III.14)$$

Only the two-pair excitation amplitude S_2 contributes to this expression. Since

$$S_2(k_1, k_2, p_2, p_1) = \delta(k_1 + k_2 - p_2 - p_1) s(k, p, P) \quad (III.15)$$

with

$$k = \frac{1}{2}(k_1 - k_2),$$

$$p = \frac{1}{2}(p_1 - p_2),$$

$$P = p_1 + p_2 = k_1 + k_2,$$

the energy per particle is readily found to be given by the expression

$$\varepsilon = \frac{1}{\rho_0} (\Phi, H(x) \Phi) + \frac{1}{4} \int dk \int dp \int dP (p | V | k) s(k, p, P) \quad (III.16)$$

The first term is just the Hartree-Fock approximation. The second term contains all the correlation effects.

Let us now return to Eq. (III.13). For any operator $A_{\underline{m}c}$ and any two functions $\epsilon(k)$, $\epsilon(p)$, we define $eA_{\underline{m}c}$ by

$$eA_{\underline{m}c} = \sum_n \frac{1}{(n!)^2} \int dk_1 \cdots \int dk_n \int dp_n \cdots \int dp_1 \\ \times [\epsilon(k_1) + \cdots + \epsilon(k_n) - \epsilon(p_n) - \cdots - \epsilon(p_1)] \quad (\text{III.17}) \\ \times A_n(k_1, \cdots, k_n; p_n, \cdots, p_1) a^\dagger(k_n) \cdots a^\dagger(k_1) b^\dagger(p_1) \cdots b^\dagger(p_n).$$

The operator $(1/e)A_{\underline{m}c}$ is similarly defined. With this definition we have

$$[H_{\underline{m}0}, S] = e_0 S, \quad (\text{III.18})$$

$$\epsilon_0(k) = \frac{k^2}{2m} \quad \epsilon_0(p) = \frac{p^2}{2m}. \quad (\text{III.19})$$

If the expression $(e^{-S} V e^S)_{\underline{m}c}$ is considered as a functional of $V_{\underline{m}}$ and $S_{\underline{m}}$, then there is a uniquely defined term of the form $[v_{\underline{m}}, S]_{\underline{m}}$, where $v_{\underline{m}}$ is a single-particle potential. The operator $v_{\underline{m}}$ in that case is

$$v_{\underline{m}} = (e^{-S_{\underline{m}}} V_{\underline{m}} e^{S_{\underline{m}}})_{1,1}. \quad (\text{III.20})$$

A double subscript n, m denotes that part of any normal ordered operator that contains n creation operators and m annihilation operators. Equation (III.13) may now be written in the form

$$S_{\underline{m}} = -\frac{1}{e} \mathcal{V}(V_{\underline{m}}, S_{\underline{m}}), \quad (\text{III.21})$$

where

$$\begin{aligned}\epsilon(k) &= (k^2/2m) + \int dk' (k|v|k') , \\ \epsilon(p) &= (p^2/2m) + \int dp' (p|v|p') ,\end{aligned}\tag{III.22}$$

and the nonlinear functional $\mathcal{V}(V, S)$ is defined by

$$\mathcal{V}(V, S) \equiv (e^{-S} V e^S)_c - [v, S] .\tag{III.23}$$

If, on the other hand, we define some effective interaction $\mathcal{W}(V, S)$ such that

$$(e^{-S} V e^S)_c = (e^{-S} \mathcal{W} e^S)_c ,\tag{III.24}$$

then the same procedure yields a different single-particle potential

$$v = (e^{-S} \mathcal{W} e^S)_{1,1} .\tag{III.25}$$

Equation (III. 13) again takes the general form

$$S = -\frac{1}{e} \mathcal{V}(\mathcal{W}, S) ,\tag{III.26}$$

where

$$\mathcal{V}(\mathcal{W}, S) \equiv (e^{-S} \mathcal{W} e^S)_c - [v, S] .\tag{III.27}$$

The most common strategy in solving a nonlinear equation, such as Eq. (III. 21) or (III. 26), is to find a starting approximation S^0 and hope to improve it by iteration. We need conditions for the convergence of such a procedure. More generally we are looking for

the existence of a solution that lies in a bounded subset of the Banach space defined in Sec. II. Under appropriate assumptions about V and ρ_0 we must show that $(1/e)\mathcal{V}$ maps a suitable subset of that Banach space into itself and that this mapping has a fixed point. The possible success of that pursuit depends on the choice of the effective interaction $\mathcal{W}$. Soft potentials are by definition potentials for which $\mathcal{W} = V$ is appropriate. For potentials with a strong short-range repulsion and a longer range attraction, an appropriate definition of $\mathcal{W}$ and the solution of Eq. (III.24) will be discussed in Sec. V.

In closing this section, it is useful to list three relevant mathematical theorems, whose proofs can be found in the references cited.

Definition: Let $\mathcal{F}(S)$ be a continuous mapping of a subset U of the Banach space B into U . The mapping is a contraction mapping if there exists a number K , $0 \leq K < 1$, such that

$$\|\mathcal{F}(S^{(1)}) - \mathcal{F}(S^{(2)})\| \leq K \|S^{(1)} - S^{(2)}\|$$

for all $S^{(1)}$ and $S^{(2)}$ in U .

Theorem 1:¹⁰ If $\mathcal{F}(S)$ is a contraction mapping of a closed subset of B into itself, then $\mathcal{F}(S)$ has a unique fixed point that can be obtained by iteration.

Theorem 2:¹¹ If $\mathcal{F}(S)$ is a contraction mapping of an open subset of B into itself and there exists a sphere $\|S - S^0\| \leq a$ such that

$$\|\mathcal{F}(S^0) - S^0\| < (1 - K)a,$$

¹⁰ J. Cronin, Fixed Points and Topological Degree in Nonlinear Analysis (American Mathematical Society, Providence, Rhode Island, 1964), p. 141.

¹¹ Th. L. Saaty and J. Bram, Nonlinear Mathematics (McGraw-Hill Book Co., New York, 1964), p. 37.

then there exists a unique fixed point that can be obtained by iteration.

Theorem 3:^{12, 13} If $\mathcal{F}(S)$ is a continuous mapping of a convex compact subset of B into itself, then there exists a fixed point

$$S = \mathcal{F}(S) .$$

This last theorem does not provide a construction of the solution. Nevertheless it can be of quantitative practical importance if the subset in question is within a sufficiently small neighborhood of some starting approximation.

IV. Soft Potentials

The heuristic principle in this section is the assumption that V and ρ_0 are chosen such that the Hartree-Fock approximation $S = 0$ is a good starting approximation to the solution of Eq. (III. 21) and the corrections may be obtained by expansion in powers of V . The single-particle potential is given by Eq. (III. 20). It is easy to see that

$$v = \{V + [V, S_2]\}_{1,1} . \quad (IV. 1)$$

The explicit expressions are

$$(k'|v|k) = \int dp (k', p|V|p, k) \\ - \frac{1}{2} \int dk'' \int dp' \int dp'' S_2(k', k''; p', p'') (p'', p'|V|k'', k) \quad (IV. 2)$$

¹² Reference 9, p. 37.

¹³ For a discussion of compactness, see S. L. Sobolev, Applications of Functional Analysis in Mathematical Physics (American Mathematical Society, Providence, Rhode Island, 1963), p. 28.

for particles above the Fermi level, and

$$\begin{aligned} (p' | v | p) &= \int dp'' (p', p'' | V | p'', p) \\ &+ \frac{1}{2} \int dk' \int dk'' \int dp'' (p', p'' | V | k', k'') S_2(k'', k'; p'', p) \end{aligned} \quad (\text{IV.3})$$

for holes.

In order to determine the explicit form of $\mathcal{V}(V, S)$ keep in mind that

$$e^{-S} c(x) e^S = c(x) + [a(x), S] \quad (\text{IV.4})$$

and

$$e^{-S} c^+(x) e^S = c^+(x) + [b(x), S] \quad (\text{IV.5})$$

and therefore

$$\begin{aligned} e^{-S} V e^S &= V + [V, S] + \frac{1}{2} [[V, S], S] \\ &+ \frac{1}{3!} [[[V, S], S], S] + \frac{1}{4!} [[[[V, S], S], S], S] \quad (\text{IV.6}) \end{aligned}$$

Let

$$v^{(n)} \equiv \{V + [V, S_2]\}_{n,n} \quad (\text{IV.7})$$

From Eq. (III.23) it follows that

$$\mathcal{V}_2(V, S) = v_2 + [v^{(2)}, S_2] + [V, (S_3 + S_4)] \quad (\text{IV.8})$$

A single subscript n on any normal ordered operator denotes that part that creates n particle-hole pairs and contains no annihilation operators. For $n \geq 3$, the general expression is

$$\begin{aligned} \mathcal{U}_n(V, S) = & J_n(V, S_2, \dots, S_{n-1}) + [(v^{(2)} + v^{(3)}), S_n] \\ & + [V, (S_{n+1} + S_{n+2})] , \end{aligned} \quad (\text{IV.9})$$

where

$$\begin{aligned} J_n(V, S_2, \dots, S_{n-1}) = & [V, S_{n-1}]_n + \frac{1}{2} [[V, S], S]_n \\ & + \frac{1}{3!} [[[V, S], S], S]_n + \frac{1}{4!} [[[[V, S], S], S], S]_n . \end{aligned} \quad (\text{IV.10})$$

Since $v^{(n)}$ depends only on S_2 , the equations

$$S_n = -(1/e) \mathcal{U}_n(V, S) \quad (\text{IV.11})$$

are linear in S_n for $n \geq 3$.

If V is small in some sense, the system of equations (IV.11) can be solved formally by iteration. In this process, the leading term in S_n is found to be $\mathcal{O}(V^{n-1})$. We are then left with the following yet-unsolved problem.

Problem: Determine necessary and sufficient conditions on V and ρ_0 such that the subset $\|S_n\| \leq \alpha V^{n-1}$ is mapped into itself by a contraction mapping for some α with $\gamma < 1$.

If we substitute the perturbation series for S_2 into Eq. (III.16), we obtain the usual perturbation expansion for the energy per particle. In the course of this derivation, terms represented by unlinked diagrams cannot arise. It is therefore unnecessary to prove a theorem stating that they cancel.¹⁴

Pending a solution of the general convergence problem, we need some numerical indication whether a given potential is indeed

¹⁴ J. Goldstone, Proc. Roy. Soc. (London) A239, 267 (1957).

soft. It is common practice in physics to judge the convergence of a series by the ratio of the second term to the first. That is a valid procedure for geometric series; but it is easy to see from Eq. (III.15) that a comparison of the first- and second-order terms in the energy is not significant. Instead one should compare the first- and third-order contributions to the energy. Such calculations were recently done by MacKenzie¹⁵ for the Tabakin¹⁶ potential and the Elliott-Flowers¹⁷ potential.

The amplitudes S_3 and S_4 first contribute to the energy in fourth and fifth order, respectively. In first order, S_2 is given by

$$S_2 = -(1/e)V_2. \quad (\text{IV.12})$$

In that approximation the single-particle spectrum given by Eqs. (III.21), (IV.2), and (IV.3) has a gap at the Fermi level. This qualitative feature is not likely to be changed by higher order corrections.

V. Solutions for Hard Potentials

Equation (IV.11) is exact, but in this form it is useful only if we can start with some initial assumption for the term $[V, (S_{n+1} + S_{n+2})]$. If the potential contains a strong short-range repulsion, these terms cannot be expected to be small.

In treating the operator $(e^{-S} V e^S)_C$ the basic rule may be stated as:

Thou shalt not split small terms into large pieces.

While the potential itself may be large, expressions of the form

¹⁵ James MacKenzie, to be published.

¹⁶ F. Tabakin, Ann. Phys. (N.Y.) 30, 51 (1964).

¹⁷ P. Elliott and B. Flowers, Proc. Roy. Soc. (London) 229, 536 (1955).

$$\frac{1}{2} \int dx_1' \int dx_2' (x_1, x_2 | V | x_2', x_1') \psi(x_1', x_2', x_3, \dots) \quad (V.1)$$

are expected to be well behaved if ψ is a solution of the Schrödinger equation. Expressions of this kind should not be split into parts that are much larger than the whole. With this purpose in mind, let the operators $\chi(x_1, x_2)$ and $\underline{W}(x_1, x_2)$ be defined by

$$c(x_1) c(x_2) \Psi = e^{\underline{S}} \chi(x_1, x_2) \Phi, \quad (V.2)$$

$$\chi(x_1, x_2) = \chi_c(x_1, x_2), \quad (V.3)$$

and

$$\underline{W}(x_1, x_2) = \frac{1}{2} \int dx_1' \int dx_2' (x_1, x_2 | V | x_2', x_1') \chi(x_1', x_2'). \quad (V.4)$$

It follows from these definitions that Eq. (III.24) holds for

$$\underline{W} = \frac{1}{2} \int dx_1 \int dx_2 c^\dagger(x_2) c^\dagger(x_1) \underline{W}(x_1, x_2). \quad (V.5)$$

It is useful to define an effective two-body interaction $\tilde{\underline{V}}$ by

$$\tilde{\underline{V}} = \frac{1}{2} \int dx_1 \int dx_2 c^\dagger(x_2) c^\dagger(x_1) \underline{W}_2(x_1, x_2), \quad (V.6)$$

where the operator $\underline{W}_n(x_1, x_2)$ is that part of $\underline{W}(x_1, x_2)$ that contains n hole-creation operators. The single-particle potential is given by Eq. (III.25),

$$\underline{V} = (e^{-\underline{S}} \underline{W} e^{\underline{S}})_{1,1} = \tilde{\underline{V}}_{1,1} \quad (V.7)$$

and hence

$$(k' | v | k) = 0, \quad (V.8)$$

$$(p' | v | p) = \int dp'' (p' p'' | \tilde{V} | p'' p) \quad (V.9)$$

It is easy to verify that the hole potentials (V.9) and (IV.3) are identical. From the definition of $\underline{W}$ and $\mathcal{V}(\underline{W}, S)$ it follows that

$$\mathcal{V} = \mathcal{V}^0 + \mathcal{V}^1, \quad (V.10)$$

$$\mathcal{V}^0 = \frac{1}{2} \int dk_1 \int dk_2 a^\dagger(k_2) a^\dagger(k_1) \underline{W}(k_1, k_2), \quad (V.11)$$

$$\mathcal{V}^1 = \int dk a^\dagger(k) \int dp \{ [b(p) + \underline{S}(p)] \underline{W}(p, k) \}_c \quad (V.12)$$

$$+ \frac{1}{2} \int dp \int dp' \{ b(p) b(p') + \underline{S}(p, p') + \underline{S}(p) \underline{S}(p') \underline{W}(p', p) \}_c$$

$$+ \int dp \int dp' \underline{S}(p) \{ b(p') [\underline{W}(p', p) - \underline{W}_2(p', p)] \}_c,$$

where

$$\underline{S}(p) \equiv [b(p), \underline{S}] \quad (V.13)$$

and

$$\underline{S}(p, p') \equiv \{ b(p), [b(p')_1 \underline{S}] \}. \quad (V.13)$$

The approximations used are based on the heuristic assumption that the pair excitation amplitudes $\underline{S}_n(x_1, \dots, x_2; p_n, \dots, p_1)$ fall off rapidly outside some healing distance¹⁸ h . We are thus led to

¹⁸ L. C. Gomes, J. D. Walecka, and V. F. Weisskopf, Ann. Phys. (N.Y.) 3, 241 (1958).

the crude estimate

$$\frac{1}{\rho_0 n!(n-1)} \int dx_2 \cdots \int dx_n, \int dp_n \cdots \int dp_1 |S_n(x_1 \cdots x_n; p_n \cdots p_1)|^2$$

$$\approx (h^3 \rho_0)^{n-1} \quad (V.15)$$

We are therefore looking for solutions of Eq. (III.25) that satisfy

$$\frac{1}{\rho_0} \|S_n\|^2 \leq a \eta^{n-1} \quad (V.16)$$

for some constant a with $\eta \ll 1$.

We expect $\mathcal{V}_n^1$ to be much less than $\mathcal{V}_n^0$ on the grounds that each integration over a momentum p , $|p| \leq k_F$, that is not fixed by momentum conservation should lower the size by a factor $\sim h^3 \rho_0$.

Equation (III.24) now has the general form

$$S_n = -\frac{1}{e} \mathcal{V}_n^0(W_n) - \frac{1}{e} \mathcal{V}_n^1(W, S), \quad (V.17)$$

where the first term is considered to be dominant. Since $\underline{W}$ is not known, we must return to Eq. (V.4) and eliminate V in favor of reaction matrices.

The reaction matrix $G(\omega)$ is a two-body matrix defined by the equation

$$G(\omega) = [1 + VQ(H_0 - \omega)^{-1}]^{-1} V, \quad (V.18)$$

where ω is a parameter and Q is a two-body projection operator into states in which both particles are above the Fermi level. The definition (V.18) leads directly to the identity

$$[1 + VQ(H_0 - \omega)^{-1}]^{-1} = 1 - G(\omega)Q(H_0 - \omega)^{-1}. \quad (V.19)$$

The potential is eliminated in favor of the reaction matrix by multiplying Eq. (V.4) by (V.19). The result is

$$\begin{aligned}
 \underline{W}(\underline{x}_1, \underline{x}_2) &= \frac{1}{2} \int d\underline{k}_1 \int d\underline{k}_2 (\underline{x}_1, \underline{x}_2 | G(\omega) | \underline{k}_2, \underline{k}_1) \frac{1}{\epsilon(\underline{k}_1) + \epsilon(\underline{k}_2) - \omega} \\
 &\quad \times \underline{W}(\underline{k}_2, \underline{k}_1) \\
 &= \frac{1}{2} \int d\underline{x}_1' \int d\underline{x}_2' (\underline{x}_1, \underline{x}_2 | G(\omega) | \underline{x}_2', \underline{x}_1') (e^{-\underline{S}} c(\underline{x}_1') c(\underline{x}_2') e^{\underline{S}})_c \\
 &= \frac{1}{2} \int d\underline{p}_1 \int d\underline{p}_2 (\underline{x}_1, \underline{x}_2 | G(\omega) | \underline{p}_2, \underline{p}_1) b^+(\underline{p}_1) b^+(\underline{p}_2) \\
 &\quad + \frac{1}{2} \int d\underline{k} \int d\underline{p} (\underline{x}_1, \underline{x}_2 | G(\omega) | \underline{p}_1, \underline{k}) \underline{S}(\underline{k}) b^+(\underline{p}) \\
 &\quad + \frac{1}{2} \int d\underline{k} \int d\underline{k}' (\underline{x}_1, \underline{x}_2 | G(\omega) | \underline{k}, \underline{k}') \underline{S}(\underline{k}') \underline{S}(\underline{k}) \\
 &\quad + \frac{1}{2} \int d\underline{k} \int d\underline{k}' (\underline{x}_1, \underline{x}_2 | G(\omega) | \underline{k}, \underline{k}') \underline{S}(\underline{k}', \underline{k}) , \tag{V.20}
 \end{aligned}$$

where

$$\underline{S}(\underline{k}) \equiv [a(\underline{k}), \underline{S}] , \tag{V.21}$$

$$\underline{S}(\underline{k}', \underline{k}) \equiv \{a(\underline{k}) [a(\underline{k}') \underline{S}]\} . \tag{V.22}$$

Equation (V.21) is used to obtain $\underline{W}$ as a functional of G and $\underline{S}$. Then according to Eq. (V.17) $\underline{S}(\underline{k}', \underline{k})$ is given by

$$\underline{S}(\underline{k}', \underline{k}) = - \frac{1}{\epsilon(\underline{k}') + \epsilon(\underline{k}) + e} [\mathcal{V}^0(\underline{k}', \underline{k}) + \mathcal{V}^1(\underline{k}', \underline{k})] , \tag{V.23}$$

where

$$\mathcal{V}(k', k) \equiv \{a(k), [a(k'), \mathcal{V}]\} \quad (V.24)$$

Keep in mind the definition $\mathcal{V}^0$, Eq. (V.11), and the expectation that $\mathcal{V}^1$ contributes only a small correction. Notice that

$$\mathcal{V}_2^0(k', k) = W_2(k', k) \quad (V.25)$$

but that $\mathcal{V}_n^1(k', k) - W_n(k', k)$ does not vanish for $n > 2$.

For $n = 2$, the second term on the left-hand side is canceled if $\omega = -e$. For $n > 2$, there is still a partial cancellation. We therefore have

$$\begin{aligned} W_2(x_1, x_2) &= \frac{1}{2} \int dp_1 \int dp_2 (x_1, x_2 | G(-e) | p_1, p_2) \\ &- \frac{1}{2} \int dk \int dk' (x_1, x_2 | G(-e) | k, k') \frac{1}{\epsilon(k) + \epsilon(k') + e} \mathcal{V}_2^1(k', k) \end{aligned} \quad (V.26)$$

and, for $n \geq 3$,

$$\begin{aligned} &W_n(x_1, x_2) + \frac{1}{2} \int dk \int dk' (x_1, x_2 | G(-e) | k, k') \\ &\times \frac{1}{\epsilon(k) + \epsilon(k') + e} (\mathcal{V}_n^0(k', k) - W_n(k', k)) \\ &= \int dk \int dp (x_1, x_2 | G(-e) | p, k) S_{n-1}(k) b^+(p) \\ &+ \frac{1}{2} \int dk \int dk' (x_1, x_2 | G(-e) | k, k') \left(S(k') S(k) \right)_n \\ &+ \frac{1}{2} \int dk \int dk' (x_1, x_2 | G(-e) | k, k') \frac{1}{\epsilon(k') + \epsilon(k) + e} \mathcal{V}_n^1(k', k). \end{aligned} \quad (V.27)$$

The Brueckner approximation is obtained if we retain only the first term in Eq. (V.26). The Bethe three-body corrections are obtained by neglecting $\mathcal{V}_3'$ and solving Eq. (V.27) for the case $n=3$. Then according to Eq. (V.12), the operator $\mathcal{V}_2'$ is given approximately by

$$\mathcal{V}_2' = \int dk a^\dagger(k) \int dp [b(p), W_3(p, k)] \quad (V.28)$$

This procedure is the beginning of a systematic algorithm. In order to ascertain the convergence, we examine the general fixed-point problem, Eq. (V.17). Since Eqs. (V.26) and (V.27) cannot be solved explicitly, we must consider a larger space of unknown functions than before. A convenient choice is to take the functionals R and Y defined by

$$R = -(1/e) \mathcal{V}' \quad (V.29)$$

and

$$Y = S - R \quad (V.30)$$

For fixed R and S , the solution of the linear equations (V.26) and (V.27) gives $W(x_1, x_2)$ as a functional of S and R or Y and R . That is,

$$W = W(Y, R) \quad (V.31)$$

We substitute that functional in Eqs. (V.11) and (V.12) and obtain

$$\begin{aligned} Y &= -\frac{1}{e} \mathcal{V}^0(Y, R) \equiv M(Y, R) , \\ R &= -\frac{1}{e} \mathcal{V}'(Y, R) \equiv N(Y, R) . \end{aligned} \quad (V.32)$$

Note that the leading term in $\mathcal{U}_2^0$ is given by the reaction matrix and is independent of $\underline{Y}$ and $\underline{R}$. We consider the set $(\underline{Y}, \underline{R}) \equiv \underline{X}$ as an element in a Hilbert space with the norm $\|\underline{X}\|$ defined by

$$\|\underline{X}\|^2 = \|\underline{Y}\|^2 + \|\underline{R}\|^2. \quad (\text{V. 33})$$

Heuristic considerations, Eqs. (V.15) and (V.16), suggest that the mapping (V.32) maps the set

$$\|\underline{Y}_n\|^2 \leq \alpha \eta^{n-1}, \quad (\text{V. 34})$$

$$\|\underline{R}_n\|^2 \leq \alpha \eta^{n+1}$$

into itself for some constant α . They also indicate that

$$\begin{aligned} & \sum_n (\|\underline{M}_n - \underline{M}_n'\|^2 + \|\underline{N}_n - \underline{N}_n'\|^2) \\ & \leq \beta \eta \sum_n (\|\underline{Y}_n - \underline{Y}_n'\|^2 + \|\underline{R}_n - \underline{R}_n'\|^2) \end{aligned} \quad (\text{V. 35})$$

for some constant β and all $\underline{Y}, \underline{R}$ that satisfy Eq. (V.34). If $\beta \eta < 1$, then the mapping (V.32) is a contraction mapping.

Problem: Determine necessary and sufficient conditions on $\underline{V}$ for $\beta \eta < 1$.

VI. The Ground State of a Closed-Shell Nucleus

The purpose of this section is to show that the ground state of a closed-shell nucleus can be obtained by the methods discussed in previous sections and to exhibit the lowest order formal approximations. The unperturbed state Φ is a single Slater determinant. The problem of determining the single-particle orbitals is the main

new feature. The occupied states will be labeled by an index ν and the empty states by ρ . In the absence of translational invariance, we have in general $S_{\mu 1} \neq 0$. It is essential for the success of the approximations to choose the single-particle orbitals in Φ such that $S_{\mu 1}$ is small. That is a reasonable expectation if $\rho_0(x)$ is a reasonable approximation to the observed density distribution. Oscillator functions or Woods-Saxon wave functions should be satisfactory for the proper choice of their parameters,

The Hamiltonian is the same as before, namely

$$H_{\mu} = H_{\mu 0} + V_{\mu}, \quad (\text{VI.1})$$

where $H_{\mu 0}$ is the kinetic energy. It is not necessary to isolate a zero-order Hamiltonian of which Φ is an eigenvector. The equation to be solved is again

$$(e^{-S_{\mu}} H_{\mu} e^{S_{\mu}})_c = 0. \quad (\text{VI.2})$$

and the ground-state energy E is

$$E = (\Phi, e^{-S_{\mu}} H_{\mu} e^{S_{\mu}} \Phi). \quad (\text{VI.3})$$

For soft potentials the Hartree-Fock approximation is obtained from the first-order perturbation term for $S_{\mu 1}$, namely

$$S_{\mu 1} = -(1/e) H_{\mu 1}. \quad (\text{VI.4})$$

Since the state

$$\Phi' = e^{S_{\mu 1}} \Phi \quad (\text{VI.5})$$

is again a single Slater determinant, formed with the functions

$$\chi_v(x) = \phi_v(x) + S(x;v) , \quad (VI.6)$$

it is possible to find single-particle orbitals such that $S_1 = 0$. They are the self-consistent Hartree-Fock orbitals.

For hard potentials the effective interactions $\underline{W}$ and $\underline{\tilde{V}}$ are defined as in Eqs. (V.5) and (V.6). Equation (VI.2) may be written in the form

$$\begin{aligned} & [(\underline{H}^0 + v), \underline{S}]_n + (\underline{H}_0)_n + \underline{V}^0(\underline{W})_n + \underline{V}^1(\underline{W}, \underline{S})_n \\ & + [\underline{H}_0, \underline{S}_{n+1}]_n + \frac{1}{2} [[\underline{H}_0, \underline{S}] \underline{S}]_n = 0 , \end{aligned} \quad (VI.7)$$

where the single-particle energy $\underline{H}^0 + v$ is given by $\underline{H}^0 = (\underline{H}_0)_{1,1}$ and

$$v = \underline{\tilde{V}}_{1,1} = - \sum_{\nu, \nu'} b^\dagger(\nu') \sum_{\nu''} (\nu, \nu'' | \underline{\tilde{V}} | \nu'', \nu') b(\nu') . \quad (VI.8)$$

The operators $\underline{V}^0$ and $\underline{V}^1$ are defined as in Eqs. (V.11) and (V.12) with the formal substitution $k \rightarrow \nu$ and $p \rightarrow \rho$.

We discuss only the lowest formal approximation to Eq. (VI.7) for $n = 1$ and $n = 2$. The last two terms and $\underline{V}_2^1$ are neglected. By definition, $\underline{V}_1^0$ and $(\underline{H}_0)_2$ vanish. In $\underline{V}_1^1$ we neglect the term arising from $\underline{W}_3$.

For any operator $\underline{A}_C$ that is a functional of creation operators only, we define

$$e \underline{A}_C = [(\underline{H}^0 + v), \underline{A}_C] . \quad (VI.9)$$

This definition implies the definition of $(1/e) \underline{A}_C$ and $f(e) \underline{A}_C$ for functions

of e . We are then left with S_1 and S_2 given by the equations

$$S_1 = -(1/e) (H_0 + \tilde{V})_1^{-1}, \quad (VI.10)$$

and

$$S_2 = -(1/e) \tilde{V}_2. \quad (VI.11)$$

As before, we use the definition of W_2 to eliminate the potential V in favor of the two-body reaction matrix $G(\omega)$ defined by

$$G(\omega) = [1 + VQ(H^0 - \omega)^{-1}]^{-1} V. \quad (VI.12)$$

We determine $W_2(x_1, x_2)$ as in Eq. (V.17) and use Eq. (VI.8) in order to find

$$\begin{aligned} W_2(x_1, x_2) &= \frac{1}{2} \sum_{\nu_1, \nu_2} (x_1, x_2 | G(-e) | \nu_2, \nu_1) b^\dagger(\nu_1) b^\dagger(\nu_2) \\ &+ \sum_{\nu \rho} (x_1, x_2 | G(-e) | \nu, \rho) S_1(\rho) b^\dagger(\nu). \end{aligned} \quad (VI.13)$$

If we substitute Eq. (VI.11) into Eq. (VI.9), we obtain a linear equation for S_1 that can be solved. Improved single-particle functions and a better Φ may be constructed from orthonormal linear combinations of the functions $\chi_\nu(x)$. For $S_1 = 0$ we give explicit expressions for $\tilde{V}$ and S_2 in the Brueckner approximation. Let $(\nu | X | \alpha)$ be the nonsingular matrix that diagonalizes the single-hole energy $(\nu | H_0 + v | \nu')$. Then

$$\sum_{\nu'} (\nu | H_0 + v | \nu') (\nu' | X | \alpha) = (\nu | X | \alpha) \epsilon_\alpha. \quad (VI.14)$$

From Eqs. (VI.13) and (VI.11) it follows that

$$\begin{aligned}
 (x_1, x_2 | \tilde{V} | \nu_2, \nu_1) &= \frac{1}{2} \sum_{\nu_1'} \sum_{\nu_2'} \sum_{\alpha\beta} (x_1, x_2 | G(\epsilon_\alpha + \epsilon_\beta) | \nu_2', \nu_1') \\
 &\times (\nu_1' | X | \alpha) (\alpha | X^{-1} | \nu_1) (\nu_2' | X | \beta) (\beta | X^{-1} | \nu_2) \quad (VI.15) \\
 &\equiv (x_1, x_2 | G | \nu_2, \nu_1) ,
 \end{aligned}$$

and

$$\begin{aligned}
 S_2(\rho_1 \rho_2; \nu_2, \nu_1) &= -\frac{1}{2} \sum_{\nu_1'} \sum_{\nu_2'} \sum_{\alpha\beta} (\rho_1 \rho_2 | \frac{1}{H^0 - \epsilon_\alpha - \epsilon_\beta} G(\epsilon_\alpha + \epsilon_\beta) | \nu_2', \nu_1') \\
 &\times (\nu_1' | X | \alpha) (\alpha | X^{-1} | \nu_1) (\nu_2' | X | \beta) (\beta | X^{-1} | \nu_2) . \quad (VI.16)
 \end{aligned}$$

The single-hole potential v and the energy E are given by

$$(v | v | \nu') = \sum_{\nu''} (v \nu'' | G | \nu'', \nu') , \quad (VI.17)$$

and

$$E = \sum_{\nu} (\nu | H_0 | \nu) + \frac{1}{2} \sum_{\nu \nu'} (v \nu' | G | \nu', \nu) . \quad (VI.18)$$

VII. The Shell-Model Problem

The purpose of this section is to apply the methods developed in previous sections to the formulation of the shell-model problem and the derivation of shell-model procedures. In this context the shell-model problem is the problem of finding the stationary states of a nucleus that differs from a closed-shell nucleus by a few nucleons or holes. Shell-model procedures solve this problem in two steps.

The first step determines an effective Hamiltonian that acts in an appropriately chosen small subspace of the full Hilbert space. The second step diagonalizes the energy matrix in that subspace.

Since we are now dealing with sets of states rather than a single state, the generalization of previously developed methods is not entirely trivial. It is useful to summarize first some elementary linear algebra and then examine the many-body features of the problem.¹⁹

Let $\mathcal{P}$ be a projection operator with the following property that there exists a set $\{\Psi_\alpha\}$ of eigenfunctions of the Hamiltonian H , such that the vectors $\mathcal{P}\Psi_\alpha$ are linearly independent and complete in the subspace defined by $\mathcal{P}$. Let F be an operator with the properties

$$F = \mathcal{P} + (1 - \mathcal{P})F\mathcal{P} \quad (\text{VII. 1})$$

and

$$HF = Fh. \quad (\text{VII. 2})$$

Our assumptions about $\mathcal{P}$ assure the existence of such an operator F .

The operator h is an effective Hamiltonian of sorts. It is defined by Eq. (VII. 2); hence

$$h = \mathcal{P}HF\mathcal{P}. \quad (\text{VII. 3})$$

The eigenvalues of h are eigenvalues of the Hamiltonian H . For if

$$h|a\rangle = |a\rangle \epsilon_a, \quad (\text{VII. 4})$$

then

$$H F|a\rangle = F|a\rangle \epsilon_a. \quad (\text{VII. 5})$$

¹⁹C. Bloch, Nucl. Phys. 6, 329 (1958); C. Bloch and J. Horowitz, Nucl. Phys. 8, 91 (1958).

The eigenfunctions $|a\rangle$ of h thus determine the corresponding eigenfunctions of H . Of course, the operator h is not Hermitian and the vectors $|a\rangle$ are not mutually orthogonal.

Let $\langle \bar{a}|$ be a dual set such that

$$\sum_a |a\rangle \langle \bar{a}| = \mathcal{P}. \quad (\text{VII. 6})$$

Then a formal solution of Eq. (VII. 2) for QF may be written in the form

$$QF = - \sum_a (QH Q - \epsilon_a)^{-1} QH |a\rangle \langle \bar{a}|, \quad (\text{VII. 7})$$

where $Q \equiv 1 - \mathcal{P}$.

It is always possible to construct a Hermitian effective Hamiltonian

$$H_{\text{eff}} = U^\dagger H U, \quad (\text{VII. 8})$$

where U is the partial isometry, defined by

$$U = F(F^\dagger F)^{-\frac{1}{2}}. \quad (\text{VII. 9})$$

Obviously U satisfies the relation

$$U^\dagger U = \mathcal{P}. \quad (\text{VII. 10})$$

The effective Hamiltonian H_{eff} is related to h by

$$H_{\text{eff}} = (F^\dagger F)^{\frac{1}{2}} h (F^\dagger F)^{-\frac{1}{2}}. \quad (\text{VII. 11})$$

The eigenfunctions

$$\phi_a = (F^\dagger F)^{\frac{1}{2}} |a\rangle \quad (\text{VII. 12})$$

are orthonormal.

In the application to the shell model, H_{eff} is the shell-model Hamiltonian and the ϕ_a are the shell-model wave functions. If these model wave functions are to be used for the calculation of transition matrix elements of some operator X , then an effective transition operator

$$X_{\text{eff}} = U^\dagger X U \quad (\text{VII. 13})$$

is required.

Let us proceed to the shell-model problem for one particle outside a closed shell. Assume that the ground state

$$\Psi = e^{\underline{S}} \Phi, \quad (\text{VII. 14})$$

$$\underline{H} \Psi = \underline{E}_0 \Psi, \quad (\text{VII. 15})$$

is known and that the state Φ has been determined such that $\underline{S}_1 = 0$.

The single-particle projection operator Λ is thus fixed, but the choice of a basis is still available in the space of the unoccupied orbitals. Let $\{\phi_p(x)\}$ be any such basis. The projection operator $\mathcal{P}$ projects into the space spanned by the basis $\{\Phi_p\}$ defined by

$$\Phi_p \equiv a^\dagger(p) \Phi. \quad (\text{VII. 16})$$

The operator $\underline{F}$ may then be written in the form

$$\underline{F} = e^{\underline{S}} \left(1 + \sum_p \underline{F}(p) a(p) \right) \mathcal{P}. \quad (\text{VII. 17})$$

The operators $\underline{F}(p)$ describe the polarization of the core by one extra particle. They create one particle and any number of particle-hole pairs, that is

$$F(\rho) = \sum_n F_n(\rho), \quad (\text{VII. 18})$$

where $F_n(\rho)$ creates one particle and n pairs.

The Schrödinger equation (VII. 2) may then be written as

$$e^{-S}(H - E_0) e^S A^+(\rho) \Phi = \sum_{\rho'} A^+(\rho') \Phi(\rho' | h | \rho), \quad (\text{VII. 19})$$

where

$$A^+(\rho) \equiv a_\rho^+ + F(\rho). \quad (\text{VII. 20})$$

Equation (VII. 19) implies the equations

$$(\Phi_{\rho'}, e^{-S}(H - E_0) e^S A^+(\rho) \Phi) = (\rho' | h | \rho)$$

and

$$\left((e^{-S}(H - E_0) e^S A^+(\rho)) \right)_n = \sum_{\rho'} F_n(\rho') (\rho' | h | \rho). \quad (\text{VII. 22})$$

Equations (VII. 21) and (VII. 22) determine simultaneously the polarization amplitudes F_n and the energy matrix h . The eigenvalues and eigenfunctions are then found by diagonalizing h .

For soft potentials, perturbation solutions of Eqs. (VII. 21) and (VII. 22) can be obtained readily. For hard potentials, the general strategy is the same as before. The analog of the operator $W(x_1, x_2)$ defined in Eq. (V. 4) is

$$U(x_1, x_2; \rho) = \frac{1}{2} \int dx_1' \int dx_2' (x_1, x_2 | V | x_2', x_1') [e^{-S} c(x_1') c(x_2') e^S, A^+(\rho)]_c. \quad (\text{VII. 23})$$

The operator U is that part of U that contains exactly n hole-creation operators.

For the left-hand side of Eq. (VII.22), we find

$$\left(e^{-\underline{S}} (H - E_0) e^{\underline{S}} A^+(\rho) \right)_n = \left[(\underline{H}_0 + \underline{V}), F_n(\rho) \right] + \mathcal{V}_n^0(\rho) + \mathcal{V}_n^1(\rho), \quad (\text{VII.24})$$

where

$$\mathcal{V}_n^0(\rho) = \frac{1}{2} \sum_{\rho_1, \rho_2} a^+(\rho_1) a^+(\rho_2) \underline{U}_n(\rho_2, \rho_1; \rho), \quad (\text{VII.25})$$

$$\begin{aligned} \mathcal{V}_n^1(\rho) = & \sum_{\rho', \nu} \{ a^+(\rho') [b(\nu) + \underline{S}(\nu)] \underline{U}_n(\nu, \rho'; \rho) \}_n \\ & + \frac{1}{2} \sum_{\nu', \nu} \{ [b(\nu)b(\nu') + \underline{S}(\nu, \nu') + \underline{S}(\nu)\underline{S}(\nu')] \underline{U}_n(\nu', \nu; \rho) \}_n \\ & + \sum_{\nu', \nu} \{ \underline{S}(\nu) b(\nu') \underline{U}_n(\nu', \nu; \rho) \}_n. \end{aligned} \quad (\text{VII.26})$$

According to the definition (VII.23), we have

$$\begin{aligned} \underline{U}_1(x_1, x_2; \rho) = & \sum_{\nu} (x_1, x_2 | \underline{V} | \rho, \nu) b^+(\nu) \\ & + \frac{1}{2} \sum_{\rho_1, \rho_2} (x_1, x_2 | \underline{V} | \rho_1, \rho_2) \underline{F}(\rho_2, \rho_1; \rho). \end{aligned} \quad (\text{VII.27})$$

It is convenient to define an effective interaction operator $\widetilde{\underline{V}}$ by

$$\widetilde{\underline{V}} = \frac{1}{2} \int dx_1 \int dx_2 \sum_{\rho} c^+(x_2) c^+(x_1) \underline{U}_1(x_1, x_2; \rho) a(\rho), \quad (\text{VII.28})$$

$$\underline{U}_1(x_1, x_2; \rho) = \sum_{\nu} (x_1, x_2 | \widetilde{\underline{V}} | \rho, \nu) b^+(\nu).$$

From Eq. (VII.20) it follows that

$$(\rho' | \underline{h} | \rho) = (\rho' | H_0 | \rho) + \sum_{\nu} (\rho', \nu | \widetilde{\underline{V}} | \nu, \rho). \quad (\text{VII.29})$$

We solve Eq. (VII.22) for $n = 1$ only and neglect $\mathcal{V}_1'$.

We are then left with the equations

$$\begin{aligned} [(H^0 + \mathcal{V}), F(\rho)] - \sum_{\rho'} F_1(\rho') (\rho' | h | \rho) \\ + \frac{1}{2} \sum_{\rho_1, \rho_2} a^+(\rho_2) a(\rho_1^+) U_{11}(\rho_1, \rho_2; \rho) = 0. \end{aligned} \quad (\text{VII. 30})$$

Equations (VII.27) — (VII.30) must be solved simultaneously. As before, we eliminate the potential $\mathcal{V}$ from (VII.27) in favor of the reaction matrix $G(\omega)$ defined in Eq. (VI.10). For fixed h and U_{11} , Eq. (VII.30) is a linear equation for F_1 that can be solved. The solution is inserted into (VII.27). For the explicit solution we need the matrix $(\nu | X | \alpha)$ defined in Eq. (VI.14) and the matrix $(\rho | Y | \delta)$ that diagonalizes h , i.e., that satisfies

$$\sum_{\rho'} (\rho | h | \rho') (\rho' | Y | \delta) = (\rho | Y | \delta) \epsilon_\delta. \quad (\text{VII. 31})$$

The operator $F_{11}(\rho)$ is related to its amplitude by

$$F_{11}(\rho) = \frac{1}{2} \sum_{\rho_1, \rho_2, \nu} a^+(\rho_2) a^+(\rho_1) b^+(\nu) F_1(\rho_1, \rho_2, \nu; \rho). \quad (\text{VII. 32})$$

The solution is then

$$\begin{aligned} (x_1, x_2 | \tilde{V} | \rho, \nu) &= \sum_{\rho' \nu'} \sum_{\alpha \delta} (x_1, x_2 | G(\epsilon_\alpha + \epsilon_\delta) | \rho', \nu') (\rho' | Y | \delta) (\delta | Y^{-1} | \rho) \\ &\times (\nu' | X | \alpha) (\alpha | X^{-1} | \nu) = (x_1, x_2 | G | \rho, \nu), \end{aligned} \quad (\text{VII. 33})$$

$$F_1(\rho_1, \rho_2, \nu; \rho) = - \sum_{\rho', \nu'} \sum_{\alpha, \delta} (\rho_1, \rho_2 | \frac{1}{H^0 - \epsilon_\alpha - \epsilon_\delta} G(\epsilon_\alpha + \epsilon_\delta) | \rho', \nu') \\ \times (\rho | Y | \delta) (\delta | Y^{-1} | \rho) (\nu' | X | \alpha) (\alpha | X^{-1} | \nu) . \quad (\text{VII. 34})$$

Equations (VII.29), (VII.31), and (VII.33) are a nonlinear set of equations for ϵ_δ and Y that must be solved by some iteration approximation.

According to Eq. (VII.11), orthonormal shell-model orbitals

$$\phi_\delta(x) = \sum_{\rho, \rho'} \phi_\rho(x) (\rho | Y^{\frac{1}{2}} | \rho') (\rho' | Y | \delta) , \quad (\text{VII. 35})$$

where

$$(\rho | Y | \rho') = \delta_{\rho, \rho'} + (\Phi, F_{\mu 1}^+(\rho') F_{\mu 1}(\rho, \Phi)) . \quad (\text{VII. 36})$$

In the treatment of two particles outside a closed shell, the one-particle problem is assumed to be solved. The model space is now spanned by the basis vectors $a^+(\delta_1) a^+(\delta_2) \Phi$, where δ_1 and δ_2 are restricted to a finite number of low-lying orbitals—for instance the d-s shell. Single-particle orbitals above the model space will be labeled by an index λ ; the index ρ labels a single-particle orbital that is anywhere above the Fermi level.

The operator $F_{\mu 1}$ may be written in the form

$$F_{\mu 1} = e^{\sum_{\mu} \frac{1}{2}} \sum_{\delta_1, \delta_2} [A^+(\delta_1) A^+(\delta_2) + C(\delta_1, \delta_2) \\ + F(\delta_1, \delta_2)] a(\delta_2) a(\delta_1) \rho , \quad (\text{VII. 37})$$

where $C(\delta_1, \delta_2)$ creates two particles of which at least one is outside the model space and the operator $F(\delta_1, \delta_2)$ describes the correlated part of the core polarization.

An effective two-body interaction $\tilde{v}$ is defined by

$$\tilde{v} = (e^{-S} H F)_{2,2} \quad (\text{VII. 38})$$

and the model energy h is then

$$h = \sum_{\delta} a^{\dagger}(\delta) \epsilon_{\delta} a(\delta) + \frac{1}{4} \sum_{\delta_1, \delta_2} \sum_{\delta_1', \delta_2'} a^{\dagger}(\delta_2') a^{\dagger}(\delta_1') (\delta_1', \delta_2' | \tilde{v} | \delta_2, \delta_1) a(\delta_1) a(\delta_2) \quad (\text{VII. 39})$$

In the lowest approximation,²⁰ the operator $F(\delta_1, \delta_2)$ is neglected and $C(\delta_1, \delta_2)$ is determined from the equation

$$Q e^{-S} H F = Q e^{-S} F h P, \quad (\text{VII. 40})$$

where the projection operator P projects into the model space, while Q projects into the space spanned by the basis $\{a^{\dagger}(\lambda) a^{\dagger}(\rho) \Phi\}$. Then to first order in the reaction matrix $G(\omega)$ given by

$$G(\omega) = [1 + VQ(QH^0Q - \omega)^{-1}]^{-1} V, \quad (\text{VII. 41})$$

the approximate solution is

$$C(\lambda, \rho; \delta_1, \delta_2) = -(\lambda, \rho | (QH^0Q - \omega)^{-1} G(\omega) | \delta_1, \delta_2), \quad (\text{VII. 42})$$

and

²⁰ T. T. S. Kuo and G. E. Brown, Nucl. Phys. 85, 40 (1966) and A92, 481 (1967); T. T. S. Kuo, Nucl. Phys. A90, 199 (1967) and A103, 71 (1967).

$$\begin{aligned}
(\rho_1, \rho_2 | \tilde{v} | \delta_2, \delta_1) &= (\rho_1, \rho_2 | G(\omega) | \delta_2, \delta_1) \\
&+ \frac{1}{2} \sum_{\nu_1, \nu_2} S_2(\rho_1, \rho_2; \nu_2, \nu_1) (\nu_1, \nu_2 | G(\omega) | \delta_2, \delta_1) \\
&+ \mathcal{A} \sum_{\nu, \rho} (\nu, \rho | G(\omega) | \delta_2, \rho) F_1(\rho_1, \rho, \nu; \delta_1), \quad (\text{VII. 43})
\end{aligned}$$

where $\omega = \epsilon(\delta_1) + \epsilon(\delta_2)$. The symbol $\mathcal{A}$ indicates antisymmetrization with respect to ρ_1, ρ_2 and δ_1, δ_2 .

The amplitudes S_2 and F_1 are also expressed in terms of reaction matrices, but they involve a different projection operator Q and different single-particle energies.