ON THE GROUND STATES OF ATOMIC NUCLEI. I

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Submitted to JETP editor March 22, 1960

J. Exptl. Theoret. Phys. (U.S.S.R.) **39**, 639-650 (September, 1960)

A variational principle is formulated and applied to a many-particle system with two-particle interaction. The wave function is chosen in a form which permits exact account to be taken of pair correlation. Equations are obtained for one- and two-particle functions in the first approximation in the correlation. It is shown that these can easily be extended to the case of strong correlations and three-particle interactions. The results are applied to the case of the so-called nuclear matter. The equations obtained are compared with those of Brueckner.

1. FORMULATION OF THE VARIATIONAL PRINCIPLE

GREAT mathematical difficulties limit the solution of the many-body problem in its application to atomic nuclei, in particular, in the study of infinitely extended nuclear matter. In this case, it is always assumed that the methods developed for spatially infinite systems (see, for example, reference 1) can easily be extended to the case of finite systems.

Inasmuch as such an assumption is not self-evident, we shall from the beginning consider a system of finite volume, consisting of N interacting particles, and attempt to ascertain for what equilibrium density this system will be stable relative to spontaneous decrease in the volume. If we assume the interactions among the particles of the system to be given, then the total energy E will depend upon the particle density distribution $\rho(\mathbf{r})$ and the condition for stability is written as

$$\delta E/\delta\rho(\mathbf{r}) = 0 \tag{1}$$

or

$$\frac{\delta((\psi|\hat{H}|\psi) - E(\psi|\psi))}{\delta\psi^*\psi} = 0, \tag{2}$$

where E is the total energy of the system.

It is evident that such a system, as for example a stable nucleus, can exist for an infinitely long time in the ground state, and consequently (1) and (2) are satisfied for it. Similar relations are not valid for excited states.

We shall now so particularize (2) that there is a possibility of taking into account the presence of two-particle correlations in the system. In this case we shall assume that the total energy depends not only on the single-particle wave functions φ_i (Hartree-Fock), but also on the pair correlation functions χ_{ik}, and requires that

$$\delta E/\delta\varphi_i = 0, \qquad \delta E/\delta\chi_{ik} = 0. \tag{3}$$

The first of these equations leads to an equation of the Hartree-Fock type, while the second permits us to consider direct interaction of pairs of particles and to make the Hartree-Fock method more precise.

If many-particle forces act in the system and it is necessary to take into account the effect of many-particle correlations, then (1) must be written in the form*

$$\sum_{i\leqslant F}\frac{\delta E}{\delta\varphi_i}\frac{\delta\varphi_i}{\delta\rho} + \sum_{i,k\leqslant F}\frac{\delta E}{\delta\chi_{ik}}\frac{\delta\chi_{ik}}{\delta\rho} + \sum_{i,k,l\leqslant F}\frac{\delta E}{\delta\eta_{ikl}}\frac{\delta\eta_{ikl}}{\delta\rho} + \ldots = 0. \tag{4}$$

Detailed consideration of (4) leads to a system of functional equations of the type (3), which represent interlocking equations for quasi-particles, pairs, etc.

However, we note that only the relations (1) and (2) follow from general considerations of the existence of a state which is stable relative to spontaneous decrease in the volume. The system (3) imposes a set of additional restrictions in comparison with (1) and (2).

2. EQUATIONS OF THE TYPE OF THE FOCK EQUATIONS

Let us consider a system consisting of N identical fermions and limit ourselves to the case in which the Hamiltonian of the system is described in the following fashion:

*$\leq F$ denotes summation over all occupied states and $>F$ over all free states.

$$\hat{H} = -\sum_{i=1}^{N} \Delta_i + \frac{1}{2} \sum_{i,k=1}^{N} V_{ik}, \qquad V_{ik} \equiv V(\mathbf{r}_i - \mathbf{r}_k). \tag{5}$$

We choose the wave function in the form

$$\psi = (N!)^{-1/2} A \prod_{i=1}^{N} \varphi_i(\mathbf{r}_i) \prod_{i<k}^{N} \chi_{ik}(\mathbf{r}_i, \mathbf{r}_k), \tag{6}$$

where A is the operator of anti-symmetrization.

Improvement of the Fock method is necessary only in the investigation of systems in which forces appear which are large in size and small in radius.

We assume that the presence of pair correlations in the motion of the particles χ_{ik} does not lead to the formation of bound complexes inside the system. Inasmuch as we shall be interested primarily in the explanation of the consequences following from the relations (1) and (2), we limit ourselves to the case of weak correlations. Representing χ_{ik} in the form[2] $1 + f_{ik}$, we keep in (6) only the terms of first order in f_{ik}:*

$$\psi = (N!)^{-1/2} A \prod_{i=1}^{N} \varphi_i(\mathbf{r}_i) \Big(1 + \sum_{k<l} f_{kl}(\mathbf{r}_k, \mathbf{r}_l)\Big). \tag{7}$$

In what follows we shall write down some qualitative considerations in favor of a similar approximation. We note that although terms like $f_{kl}f_{ij}$ possibly do not play a role in the calculation of the binding energy of such a system as an atomic nucleus, they are evidently important for the determination of the wave functions of the quasi-particles φ_i.

In the variation, the following additional conditions are imposed:

$$\int \varphi_i^*(\mathbf{r}) \varphi_k(\mathbf{r}) d\tau = \delta_{ik},$$

$$\int \varphi_k^*(\mathbf{r}) \varphi_l^*(\mathbf{r}') \varphi_f(\mathbf{r}) \varphi_n(\mathbf{r}') (1 + f_{fn}(\mathbf{r}, \mathbf{r}')) (1 + f_{kl}^*(\mathbf{r}, \mathbf{r}')) d\tau d\tau' = C\delta_{kf}\delta_{ln}, \tag{8}$$

where i, l, f, k, n ≤ F, and C is a normalization factor.

The second of the conditions (8) follows from the fact that all the levels in the ground state up to the boundary are filled. Therefore, distortion of the wave function of the pair $\psi_{ik} = \varphi_i\varphi_k(1 + f_{ik})$, due to the account of the two-particle interaction, can lead only to the appearance of components pertaining to the free states in the expansion of ψ_{ik} in φ_1, and consequently,

$$\int \varphi_k^*(\mathbf{r}) \varphi_l^*(\mathbf{r}') \varphi_f(\mathbf{r}) \varphi_n(\mathbf{r}') f_{fn}(\mathbf{r}, \mathbf{r}') d\tau d\tau' = 0, \tag{9}$$

where k, l, f, n ≤ F, which also leads to the relation (8).

We introduce the notation

$$\psi^{(0)} = (N!)^{-1/2} A \Pi \varphi_k(\mathbf{r}_k), \tag{10}$$

$$\psi^{(1)} = (N!)^{-1/2} A \Pi \varphi_k(\mathbf{r}_k) \sum_{p<l} f_{pl}(\mathbf{r}_p, \mathbf{r}_l), \tag{11}$$

$$\psi^{(2)} = \tfrac{1}{2}(N!)^{-1/2} A \Pi \varphi_k(\mathbf{r}_k) \sum_{\substack{p<l,\, i<j \\ ij \neq pl}} f_{pl}(\mathbf{r}_p, \mathbf{r}_l) f_{ij}(\mathbf{r}_i, \mathbf{r}_j). \tag{12}$$

Then the energy of the system, in first order in f_{ik}, is equal to

$$E = (\psi^{(0)} | \hat{H} | \psi^{(0)}) + (\psi^{(1)} | \hat{H} | \psi^{(0)}) + (\psi^{(0)} | \hat{H} | \psi^{(1)}). \tag{13}$$

However, the equations for the correlation functions can be obtained only by taking into account in the energy expression terms of second order in f and the change of the normalization of the wave function of the system:

$$E = \frac{(\psi^{(0)} | \hat{H} | \psi^{(0)}) + (\psi^{(1)} | \hat{H} | \psi^{(0)}) + (\psi^{(0)} | \hat{H} | \psi^{(1)})}{1 + (\psi^{(1)} | \psi^{(1)}) + (\psi^{(0)} | \psi^{(2)}) + (\psi^{(2)} | \psi^{(0)})} + \frac{(\psi^{(0)} | \hat{H} | \psi^{(2)}) + (\psi^{(2)} | \hat{H} | \psi^{(0)}) + (\psi^{(1)} | \hat{H} | \psi^{(1)})}{1 + (\psi^{(1)} | \psi^{(1)}) + (\psi^{(0)} | \psi^{(2)}) + (\psi^{(2)} | \psi^{(0)})}. \tag{14}$$

Denoting $\varphi_k(\mathbf{r})\varphi_l(\mathbf{r}')f_{kl}(\mathbf{r}, \mathbf{r}')$ and $\varphi_k(\mathbf{r})\varphi_p \times (\mathbf{r}')\varphi_l f_{kl}(\mathbf{r}, \mathbf{r}'')$ by $\overline{kl}$ and $\overline{kpl}$, respectively, we write down the matrix elements of first order in f in the form

$$(\psi^{(0)} | \hat{H} | \psi^{(0)}) = -\sum_{k=1}^{N} (k | \Delta_k | k) + \tfrac{1}{2} \sum_{i,k} (ik | V_{ik} | Aik), \tag{15}$$

$$(\psi^{(0)} | \hat{H} | \psi^{(1)}) = \sum_{k<l} (kl | -\Delta_k - \Delta_l + Q_{kl} V_{kl} | A\overline{kl}) + \sum_{k;p<l} (kpl | V_{pk} + V_{kl} | Ak\overline{pl}), \tag{16}$$

$$(\psi^{(1)} | \hat{H} | \psi^{(0)}) = (\psi^{(0)} | \hat{H} | \psi^{(1)})^*, \tag{17}$$

where A is as before the anti-symmetrization operator, and Q_{kl} is a projection operator with the following property:

$$Q_{kl} U(\mathbf{r}\mathbf{r}') = \varphi_k(\mathbf{r})\varphi_l(\mathbf{r}')(kl | U) + \sum_{i>F} \varphi_k(\mathbf{r})\varphi_i(\mathbf{r}')(ki | U) + \sum_{j>F} \varphi_j(\mathbf{r})\varphi_l(\mathbf{r}')(jl | U) + \sum_{i,j>F} \varphi_j(\mathbf{r})\varphi_i(\mathbf{r}')(ji | U). \tag{18}$$

In the expression for the energy the operator Q_{kl} is unimportant, since the matrix element in (16) does not depend on the presence of Q. The latter appears by virtue of the anti-symmetry of the initial wave function and the symmetry of $\sum_{i,k} V_{ik}$. Actually,

*Investigation of the properties of pair correlations in the case of nuclear matter, carried out by the Brueckner method in the work of Gomes et al.,[3] has shown that for pair interaction with repulsive cores of radius 0.4×10^{-13} cm χ_{ik} depends only on $\mathbf{r}_i - \mathbf{r}_k$ and differs essentially from unity for $\mathbf{r}_i - \mathbf{r}_k \approx (1 \text{ to } 1.5) \times 10^{-13}$ cm.

$$\frac{1}{2}\sum_{i,k}^{N} V_{ik}\,\psi^{(1)} = A\prod_{k=1}^{N}\varphi_k(\mathbf{r}_k)\sum_{p<q}^{N} V_{pq} f_{pq}(\mathbf{r}_p, \mathbf{r}_q) + A\prod_{k=1}^{N}\varphi_k(\mathbf{r}_k)\sum_{\substack{i<k,\ p<q,\\ ik\neq pq}} V_{ik} f_{pq}(\mathbf{r}_p, \mathbf{r}_q). \quad (19)$$

The presence of the operator A permits us to rewrite the first term of (19) in the form

$$A\Pi\varphi_k(\mathbf{r}_k)\sum_{p<q}^{N} Q_{pq} V_{pq} f_{pq}(\mathbf{r}_p, \mathbf{r}_q),$$

which also leads to the appearance of Q_{kl} in (19). The remaining matrix elements are computed and listed in the Appendix.

Varying (14) with respect to φ^* and f*, a system of interlocking equations can be obtained which permits us to find φ and f.

We introduce the following notation: the Hartree-Fock Hamiltonian

$$H_p^{HF} = -\Delta_p + \sum_k \int d\mathbf{r}'\,\varphi_k^*(\mathbf{r}')\,V(\mathbf{r}-\mathbf{r}')\,A\varphi_k(\mathbf{r}'),$$

the Hamiltonian of Bethe-Goldstone[4]

$$H_{pq}^{BG} = -\Delta_p - \Delta_q + Q_{pq}V(\mathbf{r}-\mathbf{r}') + \sum_k \int d\mathbf{r}''\,\varphi_k^*(\mathbf{r}'')\,(V(\mathbf{r}-\mathbf{r}'') + V(\mathbf{r}'-\mathbf{r}''))\,A\varphi_k(\mathbf{r}'')$$

and the Hamiltonian

$$H_{kpq} = -\Delta_k - \Delta_p - \Delta_q + Q_{kpq}(V(\mathbf{r}-\mathbf{r}') + V(\mathbf{r}-\mathbf{r}'') + V(\mathbf{r}'-\mathbf{r}'')) + \sum_l \int d\mathbf{r}'''\,\varphi_l^*(\mathbf{r}''')\,(V(\mathbf{r}-\mathbf{r}''') + V(\mathbf{r}'-\mathbf{r}''') + V(\mathbf{r}''-\mathbf{r}'''))\,A\varphi_l(\mathbf{r}'''),$$

where Q_{kpq} is the operator which projects the function of three variables on the level k, p, q and on the level lying outside the Fermi sphere F. For ψ_{pq} we obtain*

$$H_{pq}^{BG}\psi_{pq} + \Big\{\sum_k (k\,|\,H_{kpq}\,|\,A(\overline{kpq} + \overline{kpq})) + \text{compl. conj.}\Big\} + \Big[\sum_{k<l}(kl\,|\,V_{lq} + V_{pk}\,|\,A\,\overline{kl}\,pq) + \text{compl. conj.}\Big] = \varepsilon_{pq}\psi_{pq}. \quad (20)$$

The meaning of the different terms entering into the equation is easily understood. The first term is the left side of the Bethe-Goldstone equation;[4] it describes the direct action of the pair pq moving in a self-consistent field created by the remaining particles of the system. The term in the curly brackets takes into account the effect of the direct interaction of the pairs pk and qk, moving in the self-consistent field generated by the remaining particles, on the pair pq under consideration. It is significant that this effect is described by the functions f_{pk} and f_{kq}. The last term describes the action of the remaining pairs kl on the isolated pair pq.

If all $f_{ik} = 0$ except f_{pq}, then we obtain from (20) the Bethe-Goldstone equation:[4]

$$H_{pq}^{BG}\psi_{pq} = \varepsilon_{pq}\psi_{pq}. \quad (21)$$

This corresponds to the fact[3] that the Bethe-Goldstone equation* can be obtained if the interaction of the pair under discussion is considered exactly and it is assumed that the remaining particles move independently (in the sense of an absence of correlation). Their effect on the pair is reduced to the formation of a self-consistent potential.

We now consider the equation for φ obtained by variation of (13) with respect to φ_p^*:

$$H_p^{HF}\varphi_p + \Big[\sum_k (k\,|\,H_{kp}^{BG} - \varepsilon_{kp}\,|\,A\overline{kp}) + \text{compl. conj.}\Big] + \Big\{\sum_{k<l}(kl\,|\,V_{pk} + V_{pl}\,|\,Ap\overline{kl}) + \text{compl. conj.}\Big\} = E_p\varphi_p. \quad (22)$$

The first term in (22) is the left hand side of the usual Hartree-Fock equation, since the term in the square brackets takes into account the effect of direct interaction of the particles p and k moving in a self-consistent field created by the remaining particles. We note that, as in (20) for three particles, the effect of direct interaction in (22) for two particles is determined by the function f_{kp}. Finally, the last term describes the action of the pair correlations of any two particles on the considered third particle p.

An important advantage of these equations is the comparative ease of their generalization to the case of the presence of three-particle forces or considerable pair correlations, when it is necessary to take into account some higher power of f. Actually, it is easy to write down Eq. (20) in a form in which generalization to the case of three-particle potentials is trivial. In our approximation, the three-particle function has the form

$$\psi_{ikl} = \varphi_i\varphi_k\varphi_l(1 + f_{ik} + f_{il} + f_{kl}). \quad (23)$$

With account of this formula, we can write down (20) in the form

*The complex-conjugate terms differ from those written out by the fact that the correlation functions enter at the left; for example, compl. conj. in the square brackets in (20) means

$$(\overline{kl}\,|\,V_{lq} + V_{pk}\,|\,Aklpq).$$

*It is equivalent to the equation for the t-matrix of Brueckner [see (29) in reference 4].

$$H_{pq}^{BG}\psi_{pq}+\sum_k(\varphi_k\,|\,H_{kpq}\,|\,A(\psi_{kpq}-\varphi_k\psi_{pq}))$$
$$+\sum_{k<l}[(\varphi_k\varphi_l\,|\,V_{ql}+V_{pk}\,|\,A\varphi_p\varphi_q(\psi_{kl}-\varphi_k\varphi_l))$$
$$+\text{compl. conj.}]=\varepsilon_{pq}\psi_{pq}$$
$$+(1/\varphi_p^*\varphi_q^*)\sum_k(\psi_{pq}\varphi_k-\psi_{kpq}\,|\,H_{kpq}\,|\,A\varphi_k\varphi_p\varphi_q). \qquad (24)$$

Introduction of three-particle interaction leads to an evident change in the Hamiltonian H_p^{HF}, H_{pq}^{BG}, H_{kpq}. The following equation, which is necessary for the determination of ψ_{kpq}, can be written down by analogy with (24).

Just as for (20), we write Eq. (22) in the form

$$H_p^{HF}\varphi_p+\sum_k(\varphi_k\,|\,H_{kp}^{BG}-\varepsilon_{kp}\,|\,A(\psi_{kp}-\varphi_k\varphi_p))$$
$$+\sum_{k<l}[(\varphi_k\varphi_l\,|\,V_{pk}+V_{pl}\,|\,A\varphi_p(\psi_{kl}-\varphi_k\varphi_l))$$
$$+\text{compl. conj.}]=E_p\varphi_p$$
$$+(1/\varphi_p^*)\sum_k(\varphi_k\varphi_p-\psi_{kp}\,|\,H_{kp}^{BG}-\varepsilon_{kp}\,|\,A\varphi_k\varphi_p). \qquad (25)$$

In conclusion we note that in this section we have actually dealt with quasi-single-particle functions. Actually, in accord with (22), account of correlations in first order leads to the appearance of terms which depend on momentum (of the type of the effective mass M_{eff}), and to the replacement of the two-particle interaction V by V_{eff}. We shall assume that $f_{ik}=f_{ik}^*$. Then (22) takes the form

$$\left[-\frac{1}{2}\left(\Delta\frac{1}{\mu_p^{eff}}+\frac{1}{\mu_p^{eff}}\Delta\right)\right.$$
$$\left.+\sum_k\int dr'\,\varphi_k^*(r')\,V_{kp}^{eff}(rr')\,\varphi_k(r')-E_p\right]\varphi_p(r)=0,$$

$$\frac{1}{\mu_p^{eff}}=\frac{M}{M_p^{eff}}=1+2\sum_k\int|\varphi_k(r')|^2 f_{kp}(r'r)\,dr',$$

$$V_{kp}^{eff}=V_{kp}\left\{A+f_{kp}A+Af_{kp}+\sum_l[(\varphi_l f_{lp}\,|\,\varphi_l)A\right.$$
$$+(\varphi_l\,|\,\varphi_l Af_{lp})+(\varphi_l\,|\,\varphi_l f_{kl})A+(\varphi_l\,|\,\varphi_l Af_{kl})]\Big\}$$
$$-f_{kp}(\Delta_k+\varepsilon_{pk})A-(\Delta_k+\varepsilon_{pk})Af_{kp}$$
$$+\sum_l[(\varphi_l\,|\,V_{lk}\,|\,f_{kp}A\varphi_l)+(\varphi_l\,|\,V_{lk}\,|\,Af_{kp}\varphi_l)]. \qquad (22a)$$

Hence it is clear that account of pair correlations in finite systems leads simultaneously to mass "renormalization" and two-particle interaction, while, roughly speaking, $V_{eff}/V\approx M/M_{eff}$, in accord with the fact that introduction of the effective mass requires a change in the depth of the potential well in the relation written down, as is well known.

3. NUCLEAR MATTER

An approach was developed by a number of authors to the solution of the many-body problem which is known as the Brueckner approximation, which takes pair interactions between the particles into account, in more exact fashion than in the Hartree-Fock method. Let us consider the problem of the relationship of the Brueckner method to our variational principle (22) and compare the equations of reference 1 with those obtained in the present work.

According to Brueckner, the expression for the energy of a system of particles with the Hamiltonian (5) can be described,[1] after some simplification, in the form

$$E=-\sum_{i=1}^{N}(i\,|\,\Delta\,|\,i)+\frac{1}{2}\sum_{i,k=1}^{N}(ik\,|\,t\,|\,Aik),$$
$$(ik\,|\,t\,|\,lq)=(ik\,|\,V\,|\,lq)+\sum_{s,p>F}\frac{(ik\,|\,V\,|\,sp)(sp\,|\,t\,|\,lq)}{E_l+E_q-E_s-E_p},$$
$$E_l=-(l\,|\,\Delta\,|\,l)+\sum_{q\leqslant F}(lq\,|\,t\,|\,Alq). \qquad (26)$$

In the process of constructing the Brueckner equation for finite nuclei, it is assumed that solutions of the equation

$$\Delta\varphi_i+\int(r\,|\,U\,|\,r')\,\varphi_i(r')\,d\tau'=E_i\varphi_i(r) \qquad (27)$$

form a complete set of basis functions and the self-consistent nonlocal potential is chosen from the condition of vanishing of the contribution of terms of second order in the expansion of the energy of the system in t:

$$(\varphi_i\,|\,U\,|\,\varphi_i)=\sum_{k\leqslant F}(ik\,|\,t\,|\,Aik). \qquad (28)$$

We introduce the operator R, for which t = VR, and denote $R\varphi_i\varphi_k=\psi_{ik}$. Then, inasmuch as

$$\int(r\,|\,U\,|\,r')\,\varphi_k(r')\,d\tau'=\sum_{i\leqslant F}\int\varphi_i^*(r')\,(r',\ r\,|\,t\,|\,Aik)\,d\tau',$$
$$(r,\ r'\,|\,t\,|\,Aik)=V(r-r')\,\psi_{ik}(r,\ r'), \qquad (28a)$$

we find a set of interlocking equations [by transforming in (26) to a mixed representation] which connect the one- and two-particle functions.*

$$-\Delta\varphi_i+\sum_{k\leqslant F}\int d\tau'\varphi_k^*(r')\,V(r-r')\,\psi_{ik}(r,\ r')=E_i\varphi_i,$$
$$\psi_{ik}(r,\ r')=A\varphi_i(r)\,\varphi_k(r')+\sum_{q,\ l>F}\int d\tau''d\tau'''$$
$$\times\frac{\varphi_q(r)\,\varphi_l(r')\,\varphi_q^*(r'')\,\varphi_l^*(r''')}{E_i+E_k-E_q-E_l}V(r''-r''')\,\psi_{ik}(r'',\ r'''). \qquad (29)$$

*It can be shown that the second equation of (29) coincides with the Bethe-Goldstone equation.[4]

The first equation of the set (29) is similar to the Hartree-Fock equation, but it cannot be obtained by the Fock variational principle from the equation for the energy of the system.

Actually, by varying E with respect to φ_i^*, we would have obtained the equation

$$-\Delta\varphi_i + \sum_{k\leqslant F}\int d\tau'\,\varphi_k^*(\mathbf{r}')\,V(\mathbf{r}-\mathbf{r}')\,\psi_{ik}(\mathbf{r},\mathbf{r}') + \tfrac{1}{2}\sum_{k,\,q\leqslant F}\int d\tau' d\tau''\varphi_k^*(\mathbf{r}')\,\varphi_q^*(\mathbf{r}'')\,V(\mathbf{r}'-\mathbf{r}'') \times \frac{\delta\psi_{ik}(\mathbf{r}',\mathbf{r}'')}{\delta\rho(\mathbf{r})}\frac{\delta\rho(\mathbf{r})}{\delta\varphi_i(\mathbf{r})} = E_i\varphi_i, \tag{30}$$

which differs from (29) by a term which has been given the name "rearrangement potential" in the literature.

If the wave function is determined from (30), then the initial assumption (28) is generally violated; according to this assumption one can neglect terms of second order in t and in place of (26) there would be introduced another expression for the total energy. Estimates of the term arising because of the dependence of the t-matrix on the density of nuclear matter, carried out by Brueckner,[5] show that it is approximately equal to 10-15 Mev, and consequently it cannot be neglected.

We shall now consider to what the variational principle (2) leads for the case of nuclear matter, where, as follows from general considerations connected with the absence of a singularity in the system with the Hamiltonian (5), the correlation functions $f_{ik}(\mathbf{r}_i, \mathbf{r}_k)$ depend only on the difference $\mathbf{r}_i - \mathbf{r}_k$, while the quasi-single-particle functions are plane waves. In this case, as is not difficult to show, we have in place of (9),

$$\int \varphi_k^*(\mathbf{r})\,\varphi_i(\mathbf{r})\,f_{il}(\mathbf{r},\mathbf{r}')\,d\tau = 0, \tag{31}$$

and the action of the projection operator on a function depending on the difference in the coordinates is now determined by the relation

$$Q_{kl}W(\mathbf{r}-\mathbf{r}') = \varphi_k(\mathbf{r})\,\varphi_l(\mathbf{r}')\,(kl\,|\,W) + \sum_{i,j>F}\varphi_i(\mathbf{r})\,\varphi_j(\mathbf{r}')\,(ij\,|\,W), \tag{32}$$

which takes the place of (18).

The relation (31)shows that the matrix element corresponding to graphs of the type of Fig. 1 with free ends, corresponding to correlation functions,* do not make a contribution, in the case of nuclear matter, to the expression for the total energy of the system. The latter, in accord with (15), (16), and (17), is equal to

*A description of graphical techniques is given in the Appendix.

$$E = -\sum(k\,|\,\Delta\,|\,k) + \sum_{i<k}[(ik\,|V_{ik}|\,Aik) + (ik\,|V_{ik}|\,\overline{ik}) + \text{c. c.}]. \tag{33}$$

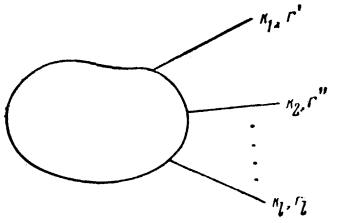

FIG. 1

This expression is essentially in agreement with (26) if we take into account (28a).

From (15), (16), (17), and (33) we find equations for φ_i and ψ_{ik} which we write in a form suitable for comparison with (29):

$$-\Delta\varphi_i + \sum_{k\leqslant F}(\varphi_k(\mathbf{r}')\,|\,V(\mathbf{r}-\mathbf{r}')(1+f_{ik}^*(\mathbf{r},\mathbf{r}'))\,|\,A\psi_{ik}(\mathbf{r},\mathbf{r}')) = E_i\varphi_i, \tag{34}$$

$$H_{ik}^{BG}\psi_{ik} = \varepsilon_{ik}\psi_{ik} - \sum_p\{(p\,|\,V_{ip}\,|\,A\overline{pik}) + (p\,|\,V_{kp}|\,A\overline{pik}) + \text{c. c.}\}. \tag{35}$$

Hugenholtz[6] has shown that the Brueckner method is valid in the approximation of small particle distribution density in the system if a number of assumptions are made whose validity is questionable. We have made use of the assumption of the smallness of the correlation functions. This is obviously equivalent to the approximation of low density,* inasmuch as the latter reduces to elimination of the possibility of simultaneous direct action of more than two particles.

However, it is seen that even in the approximation under consideration for wave functions of pairs an equation is obtained which differs somewhat from (21) [it can be shown that (21) is equivalent to (29)]. The complementary terms in (35), in comparison with (21), have a very clear physical meaning; for example, the first term in the curly brackets describes the change of the self-consistent field acting on the particle i as a result of correlations between the moving particles k and p.

It seems to us that the form of Eq. (35) strengthens the validity of the doubts raised by Hugenholtz,[6,7] inasmuch as there are no very weighty arguments for the elimination of the additional terms in (35), except for, in our view, not very convincing general remarks which reduce

*If we denote the momentum of the Fermi system by k_F and the effective radius of the two-particle interaction by r_0, then by the approximation of low density is understood an approximation which is valid for $k_F r_0 \ll 1$.

to the fact that, inasmuch as the wave function of the pair ψ_{ik} differs markedly from the product of one-particle functions only at small values of $\mathbf{r} - \mathbf{r}'$ (see reference 3), the remaining particles act on the given pair as free particles and, consequently, the term in the curly brackets in (35) should be thrown out.

Comparison of (35), (20), and (21) shows that the method developed by Brueckner is valid only for spatially infinite systems and the application of it to finite systems requires not only the replacement of quasi-one-particle functions by functions of finite systems (oscillator and so forth, as was done, for example by Banerjee and Roy,[8] and by Eden and Emery[9]) but also an important change in the fundamental equations — the substitution of (34) and (35) for (20) and (22).

4. SATURATION OF NUCLEAR FORCES AND THE VARIATIONAL PRINCIPLE (2)

It is known from experiment that the energy entering into a single nucleon in the nucleus E_{av} and the mean density of nuclear matter ρ_{av} do not depend on the number of nucleons in the nucleus N and are equal to 8 Mev and 2×10^{38} cm^{-3}, respectively. For nuclear matter, by virtue of the infinite volume of the system Ω, we have as $\Omega \to \infty$*

$$\frac{\partial E_{av}}{\partial N} = \frac{1}{\Omega}\frac{\partial E_{av}}{\partial \rho} \to 0, \qquad \frac{\partial \rho_{av}}{\partial N} = \frac{1}{\Omega} - \frac{\rho}{\Omega}\frac{\partial \Omega}{\partial N} \to 0,$$
$$(\rho = \rho_{av} = N/\Omega). \tag{36}$$

If the interaction between the particles is given, then $E = E(\rho)$ and for a fixed number of particles we have for the ground state

$$\left.\frac{\partial E}{\partial \rho}\right|_N = 0,$$

that is, $\partial E_{av}/\partial \rho = 0$ and $\partial E_{av}/\partial N = 0$ not only when $\Omega \to \infty$. It is thus seen that the requirement $\partial E_{av}/\partial \rho = 0$, which usually figures in researches on nuclear matter, follows from the condition for the existence of a stable configuration of nuclear matter which is distributed over all space with the same density. This requirement for nuclear matter coincides with the experimental observed independence of E_{av} on the number of nucleons in the nucleus.

We note that the variational principle (2) does not guarantee saturation of nuclear forces and density, for finite systems, in the sense of independence of E_{av} and ρ_{av} of the number of nucleons in the nucleus. The satisfaction of (2) speaks only of the existence of a stable state of the system with a finite number of particles in a spatially limited volume.

For example, (2) can be valid also for forces entering into the "collapse" (contraction) of nuclei. Satisfaction of the same conditions $\partial E_{av}/\partial N \approx 0$ and $\partial \rho_{av}/\partial N \approx 0$ depends on the specific character of the nuclear forces.

*The density of nuclear matter is equal to the mean density of finite nuclei.

CONCLUSION

The reliability of the approximation of weak correlation used by us depends on how the forces act between the nucleons in the nucleus. Data on nucleon-nucleon scattering in the range from 2 to 300 Mev can be interpreted with the aid of various potentials: the potentials of Signel and Marshak, of Gammel-Christian-Teller, of Gammel-Teller. The latter is widely used in the researches of Brueckner and his co-workers. The characteristic of this potential lies in the introduction of infinitely strong repulsions at small distances ($r \leq 0.5 \times 10^{-13}$ cm). In the present research, we have essentially limited ourselves to the qualitative side of the problem, not touching on the possibility of the use of Eqs. (21), (22), (33), and (34) for calculation of the ground state of a system of nucleons interacting, for example, through a Gammel-Teller potential. A more detailed investigation of the resultant equations, and also a concrete calculation will be given in a subsequent paper.

Moreover, we have assumed from the beginning that pair correlations do not lead to the formation of bound states. Bound states, for example, in infinite nuclear matter, are characterized by the fact that not $f(\mathbf{r}_1 - \mathbf{r}_2)$, but $\chi(\mathbf{r}_1 - \mathbf{r}_2) \to 0$ for $\mathbf{r}_1 - \mathbf{r}_2 \to \infty$. Therefore, account of bound pairs, say in the region of the Fermi surface, would have required for the model under consideration the use of the correlation functions χ and not f.

The impression can be created that the superposition of a large number of conditions $\delta E/\delta \chi_{ik} = 0$ makes the system redefined. However, if we assume approximately that all correlation functions are identical, then in place of $N(N-1)$ there will be only a single additional condition, and the equations (21), (22), (33), (34) are essentially unchanged. One of the achievements of the method considered is the ease of generalization to the case of strong correlations, many-particle interactions (24) and (25) of systems composed of particles of several sorts, $\alpha, \beta, \ldots$, etc.

In the latter case, it is necessary to require

$$\delta E/\delta \rho_\alpha = \delta E/\delta \rho_\beta = \ldots = 0, \qquad \delta E/\delta \varphi_i^{(\alpha)} = \delta E/\delta \varphi_i^{(\beta)} = \ldots = 0,$$
$$\delta E/\delta \chi_{ik}^{\alpha)} = \delta E/\delta \chi_{ik}^{(\beta)} = \ldots = 0. \tag{37}$$

in place of (1) and (3). Violation of (37) in the ground state of atomic nuclei leads to spontaneous conversion $-\beta^{\pm}$, α decays, and fission.

In conclusion we note that the application of the variational principle (2) to boson systems with two- and many-particle interactions makes it possible to obtain equations for them of the type (20), (22), (24) and (25).

I take it my pleasant duty to express my deep gratitude to Professor L. A. Sliv for numerous discussions and valuable remarks, and also to G. M. Sklyarevskiĭ and B. L. Birbrair for discussion of the results.

APPENDIX

For the matrix element $(\psi^{(1)} | H | \psi^{(1)})$, we find

$$(\psi^1 | \hat{H} | \psi^{(1)}) = -\sum_{p<q} (\overline{pq} | \Delta_p + \Delta_q | A\overline{pq})$$

$$-\sum_{\substack{p<q\\k\neq p,q}} (k | \Delta | k)(\overline{pq} | A\overline{pq})$$

$$-\sum_{p<q,k} (\overline{kpq} | \Delta_k + \Delta_p + \Delta_q | A\overline{kp}\,q)$$

$$-\sum_{k,p<q} (\overline{kpq} | \Delta_k + \Delta_p + \Delta_q | A\overline{kpq})$$

$$-\sum_{\substack{i\neq p,q,k\\p<q,k}} (i | \Delta | i)(\overline{kpq} | A\overline{kpq}) - \sum_{\substack{i\neq p,q,k\\k,p<q}} (i | \Delta | i)(\overline{kpq} | A\overline{kpq})$$

$$+\sum_{p<q} (\overline{pq} | V_{pq} | A\overline{pq}) + \sum_{\substack{i<k;\ p<q\\ik\neq pq}} (ik | V_{ik} | Aik)(\overline{pq} | A\overline{pq})$$

$$+\sum_{k,p<q} (\overline{kpq} | V_{kp} + V_{kq} | Ak\overline{pq})$$

$$+\sum_{\substack{i<k;\ p<q,l\\ik\neq p,q,l}} (ik | V_{ik} | Aik)(\overline{lpq} | A\overline{lp}\,q)$$

$$+\sum_{\substack{i<k;l,p<q\\i,k\neq p,q,l}} (ik | V_{ik} | Aik)(\overline{lpq} | A\overline{lpq})$$

$$+\sum_{k,\ p<q} (\overline{kpq} | V_{kp} + V_{pq} + V_{qk} | A\overline{kpq})$$

$$+\sum_{p<q,k} (\overline{kpq} | V_{kp} + V_{pq} + V_{qk} | A\overline{kp}\,q)$$

$$+\sum_{p<q,\ k<l} (\overline{kpq}\,l | V_{kl} + V_{pl} + V_{ql} | A\overline{kp}\,ql)$$

$$+\sum_{k,p<q<l} (\overline{kpq}\,l | V_{kl} + V_{pl} + V_{ql} | A\overline{kpql})$$

$$+\sum_{q<p,\ k<l} (\overline{kpq}\,l | V_{kl} + V_{pq} | Ak\overline{pql}).$$

It is convenient to associate a graph with each matrix element, introducing the corresponding graphical form for the different functions and corresponding operators entering into the expression for the matrix element. We shall denote the correlation function $f_{pl}(\mathbf{r}, \mathbf{r}')$ by a solid line directed from $\mathbf{r}'$ to $\mathbf{r}$ (see Fig. 2), the complex conjugate function $f^*_{pl}(\mathbf{r}, \mathbf{r}')$ by a solid line directed from $\mathbf{r}$ to $\mathbf{r}'$. The potential $V(\mathbf{r} - \mathbf{r}')$ will be expressed by a wavy line, and the Laplace operator Δ by a dashed line.

The matrix element

$$(\overline{kpq} | \Delta_k + \Delta_p + \Delta_q | A\overline{kpq})$$

is described by the graph of Fig. 3a, and the matrix element

$$(k\overline{pq} | V_{kp} + V_{pq} + V_{qk} | A\overline{kpq})$$

by the graph of Fig. 3b. The matrix element $(ik | V_{ik} | A_{ik})(\overline{pq} | A | \overline{pq})$ corresponds to the unconnected graph of Fig. 4.

Consideration of the matrix elements makes it possible to formulate a number of rules with whose help it is possible to construct the expression for the energy of the system of N particles with account of corrections of second, third and higher degrees in the correlation functions.

1. Graphs determining the energy of the system contain not more than $2(N-1)$ straight lines, the vertex index p and its coordinate $\mathbf{r}$ are the same for all lines entering the vertex.

2. In each graph there is not more than one wavy or dashed line.

3. Graphs with disconnected straight lines are equal to zero.

4. Summation in the expression of the energy is carried out over all indices encountered in the diagram, and integration over the coordinates of the end lines.

5. Closed loops of solid lines are possible only in those cases in which it is possible with account

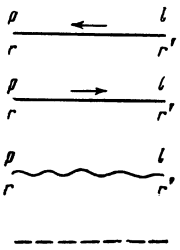

FIG. 2

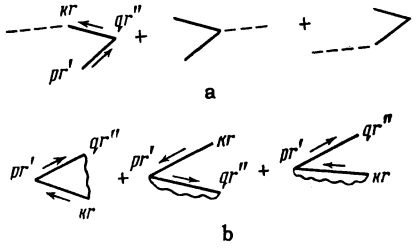

FIG. 3

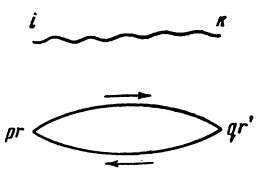

FIG. 4

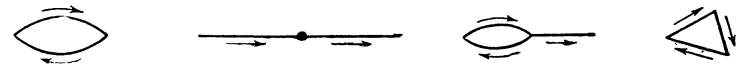

FIG. 5

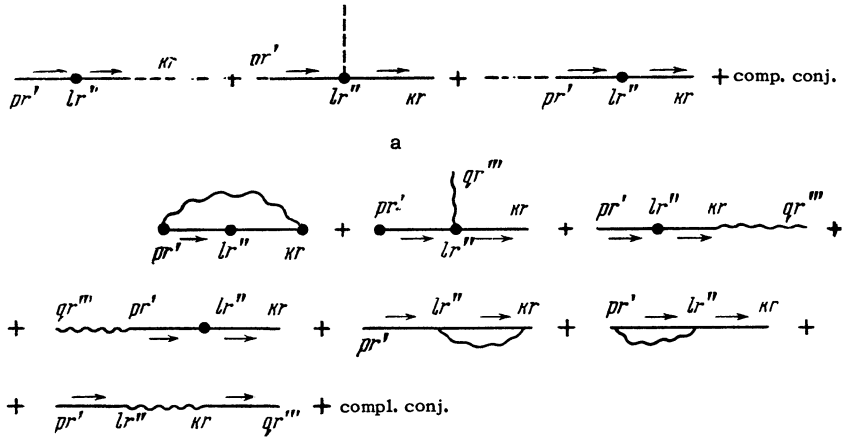

FIG. 6

of the direction of the lines to form a closed contour with a definite direction of rotation — in the clockwise direction or the reverse.

6. To each index k and coordinate $\mathbf{r}$ of the end of the line there corresponds $\varphi_k(\mathbf{r})$ and $\varphi_k^*(\mathbf{r})$. The correlation functions directed to the right and the product of all functions φ corresponding to a given graph are anti-symmetrized.

7. Graphs with unconnected wavy and dashed lines do not, in any case for large systems, make any contribution to the expression for the energy since they correspond to normalization of the complete wave function of the system.

8. If the graph consists of several disconnected parts, then summation in each part is carried out independently; however, in each term of the sum the disconnected parts do not keep the same indices.

Making use of rules 1 — 8, it is possible to establish the fact that graphs containing disconnected correlation parts of the type of Fig. 5 do not have to be taken into account in the computation of the energy since they correspond to normalization of the wave function of the ground state.

Thus, the situation here is similar to quantum field theory where the vacuum-vacuum transitions do not change the propagation function.

Higher degrees of correlation functions f take into account the change of the energy of the system as the result of finding three or more particles close to one another.

The matrix element $(\psi^{(2)}|\hat{H}|\psi^{(0)}) + (\psi^{(0)}|\hat{H}|\psi^{(2)}) = T^{(2)} + U^{(2)}$ is represented by the graph of Fig. 6 ($T^{(2)}$ corresponds to the graph of Fig. 6a; $U^{(2)}$ to the graph of Fig. 6b; we have omitted the disconnected graphs). Making use of rules 1 — 8, it is easy to write down the analytic expressions for $T^{(2)}$ and $U^{(2)}$.

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Translated by R. T. Beyer
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