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S. V. TYABLIKOV

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Abstract

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S. V. TYABLIKOV

ON A VARIATIONAL PRINCIPLE IN THE MANY-BODY PROBLEM

(Presented by Academician N. N. Bogolyubov, 12 III 1958)

In the work of N. N. Bogolyubov ([1]), a variational principle in the many-body problem was formulated. Below we formulate the condition under which a given solution of the generalized method gives a minimum of the ground-state energy; this reduces to the condition of positivity of the second variation of the expression for the ground-state energy. Since among the solutions of the generalized method there are always also solutions of the ordinary Fock method, we thereby obtain a criterion for when the ordinary Fock method does not give an energy minimum and the latter should be sought in a broader class of solutions of the generalized method.

Let the Hamiltonian of a system of N interacting Fermi particles in the second-quantization representation have the form

$$H = \sum (A(f, f') - \alpha\delta_{f,f'})\, a_f^+ a_{f'} + \frac{1}{2}\sum B(f_1, f_2; f_2', f_1')\, a_{f_1}^+ a_{f_2}^+ a_{f_2'} a_{f_1'}, \quad (1)$$

where $A(f, f')$ and $B(f_1, f_2; f_2', f_1')$ are the matrix elements of the operators of the proper energy of the particles and of the interaction energy; α is the chemical potential, introduced so as not to take explicitly into account the condition of constancy of the number of particles in the system; f is the set of indices characterizing the state of a particle. To determine α we have the usual condition

$$\sum_{(f)} \overline{a_f^+ a_f} = N. \quad (2)$$

For the matrix elements of the operators A, B, the obvious conditions hold:

$$A^*(f, f') = A(f', f); \quad B^*(f_1, f_2; f_2', f_1') = B(f_1', f_2'; f_2, f_1) = B(f_2', f_1'; f_1, f_2). \quad (3)$$

We perform a canonical transformation of the operators a:

$$a_f = \sum_{(\nu)} (u_{f\nu} a_\nu + v_{f\nu} a_\nu^+), \tag{4}$$

where the functions u, v satisfy the following orthogonality and normalization conditions:

$$\xi_{ff'} = \sum_{(\nu)} (u^*_{f\nu} u_{f'\nu} + v^*_{f\nu} v_{f'\nu}) = \delta_{ff'}; \quad \eta_{ff'} = \sum_{(\nu)} (u_{f\nu} v_{f'\nu} + u_{f'\nu} v_{f\nu}) = 0. \tag{5}$$

We now compute the mean value of H (1) with respect to the vacuum function in the new variables a_ν:

$$a_\nu c_0 = 0. \tag{6}$$

Assuming the function c_0 to be normalized, we shall have:

$$\overline{H} = \sum \left(A(f, f') - \alpha \delta_{ff'} \right) F(f, f') + \frac{1}{2} \sum G(f_1, f_2; f'_2, f'_1) F(f_1, f'_1) F(f_2, f'_2) + \frac{1}{2} \sum B(f_1, f_2; f'_2, f'_1) \Phi^*(f_1, f_2) \Phi \tag{7}$$

$$G(f_1, f_2; f'_2, f'_1) = B(f_1, f_2; f'_2, f'_1) - B(f_1, f_2; f'_1, f'_2); \tag{8}$$

$$\Phi(f_1, f_2) = \sum_{(\nu)} v_{f_1\nu} u_{f_2\nu}, \qquad F(f_1, f_2) = \sum_{(\nu)} v^*_{f_1\nu} v_{f_2\nu}, \qquad F_0(f_1, f_2) = \sum_{(\nu)} u^*_{f_1\nu} u_{f_2\nu}. \tag{9}$$

We determine u, v from the condition that the form (7) have a minimum, under the additional conditions (5):

$$\mathcal{E} = \overline{H} + \sum \lambda(f_1, f_2)(F(f_1, f_2) + F_0(f_1, f_2)) + \sum m(f_1, f_2) \Phi(f_1, f_2) + \sum m^*(f_1, f_2) \Phi^*(f_1, f_2) - \sum \lambda(f, f) = \min \tag{10}$$

where λ, m are undetermined Lagrange multipliers, and, by virtue of the second of conditions (5), $m(f_1, f_2) = m(f_2, f_1)$.

From the condition that the first variation of $\mathcal{E}$ vanish, we obtain equations for determining the functions u, v:

$$\sum_{(f_2)} (Q(f_1, f_2) + \lambda(f_1, f_2)) v_{f_2\nu} + \sum_{(f_2)} (R^*(f_2, f_1) + m^*(f_2, f_1)) u^*_{f_2\nu} = 0;$$

$$\sum_{(f_2)} \lambda(f_1, f_2) u_{f_2\nu} + \sum_{(f_2)} (R^*(f_1, f_2) + m^*(f_1, f_2)) v^*_{f_2\nu} = 0 \tag{11}$$

(and also two equations conjugate to these), where the following notation has been introduced:

$$Q(f_1, f_2) = A(f_1, f_2) - \alpha \delta_{f_1 f_2} + \sum_{(g_1, g_2)} G(f_1, g_1; g_2, f_2) F(g_1, g_2);$$

$$R(f_1, f_2) = \frac{1}{2} \sum_{(g_1, g_2)} B(g_1, g_2; f_1, f_2) \Phi^*(g_1, g_2). \tag{12}$$

Equation (2) for determining the chemical potential α, taking into account (4), (6), (9), assumes the form

$$\sum_{(f)} F(f, f) = N. \tag{13}$$

It is clear that equations (11) may be regarded as a generalization of Fock' s equations, to which they reduce under the following choice of the functions u, v:

$$u_{f\nu} = 0, \qquad v_{f\nu} = w_{f\nu}, \quad \nu \in F;$$

$$u_{f\nu} = w_{f\nu}, \qquad v_{f\nu} = 0, \quad \nu \notin F, \quad m(f_1, f_2) = 0, \tag{14}$$

where $w_{f\nu}$ is a system of functions orthonormalized in the usual sense; F is the "Fermi sphere," which is defined as the set of N indices ν (N is the number of particles). Below we shall call the solution (14) the ordinary one.

Equations (11) always have a solution of the form (14), where $w_{f\nu}$ are chosen by Fock' s method. Consequently, the limits of applicability of the new method cannot be narrower than the limits of applicability of the ordinary Fock method.

Solutions of equations (11) will be stable if they minimize the expression (10) for the energy of the system $\mathcal{E}$, i.e., if the second variation of $\mathcal{E}$

will be positive. The expression for the latter is brought to the form

$$\delta^2 \mathcal{E} = 2 \sum_{(f,\nu)} E \left(\delta v^*_{f\nu} \delta v_{f\nu} + \delta u^*_{f\nu} \delta u_{f\nu} \right), \tag{15}$$

where E, δv, δu are the eigenvalues and eigenfunctions of the equations in variations:

$$\sum_{(f_2)}(Q(f_1,f_2)+\lambda(f_1,f_2))\delta v_{f_2\nu}+\sum_{(f_2)}(R^*(f_2,f_1)+m^*(f_2,f_1))\delta u^*_{f_2\nu}$$
$$+\sum_{(g_1,g_2,f_2,\mu)}G(f_1,g_1;g_2,f_2)\left(\delta v_{g_1\mu}v^*_{g_2\mu}+v^*_{g_1\mu}\delta v_{g_2\mu}\right)v_{f_2\nu}$$
$$+\frac{1}{2}\sum_{(g_1,g_2,f_2,\mu)}B^*(g_1,g_2;f_2,f_1)\left(\delta v_{g_1\mu}u_{g_2\mu}+v_{g_1\mu}\delta u_{g_2\mu}\right)u^*_{f_2\nu}=E\delta v_{f_1\nu};\quad(16)$$
$$\sum_{(f_2)}\lambda(f_1,f_2)\delta u_{f_2\nu}+\sum_{(f_2)}(R^*(f_1,f_2)+m^*(f_1,f_2))\delta v^*_{f_2\nu}$$
$$+\frac{1}{2}\sum_{(g_1,g_2,f_2,\mu)}B(g_1,g_2;f_1,f_2)\left(\delta v_{g_1\mu}u_{g_2\mu}+v_{g_1\mu}\delta u_{g_2\mu}\right)v^*_{f_2\nu}=E\delta u_{f_1\nu}.$$

(and two more equations conjugate to these). It is evident that expression (15) will be positive if the system of equations (16) has no negative eigenvalues.

It follows from this that the usual Fock solution (14) will be stable, i.e. will give a minimum of the ground-state energy, not under all conditions. The instability of the ordinary solution (14) is naturally interpreted as a criterion for the existence in the system of some other state.

Thus, in the particular case

$$A(f_1,f_2)=A(f_1)\delta_{f_1f_2}\quad(f=(q,s));$$

$$B(f_1,f_2;f_2',f_1')=B(q_1s_1;\ q_1s_2;\ q_2's_2';\ q_2's_1')(1-\delta_{q_1q_2}),$$

where q is the momentum, and s is the totality of the coordinates of the ordinary and isotopic spins, from (16) there follows N. N. Bogolyubov' s criterion for the condition of existence of superfluidity in nuclear matter ([3]).

The new method is also very convenient for investigating various questions in the electron theory of solids with allowance for the crystal lattice, for example in establishing a criterion for superconductivity with allowance for the lattice.

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CITED LITERATURE

[1] N. N. Bogolyubov, DAN, 119, No. 2 (1958).
[2] V. A. Fock, Zs. f. Phys., 61, 126 (1930).
[3] N. N. Bogolyubov, DAN, 119, No. 1 (1958).

Note: Figure translations are in progress. See original paper for figures.