

309

JOINT INSTITUTE FOR NUCLEAR RESEARCH

Laboratory of Theoretical Physics

V.G.Soloviev

P.309

EQUATION FOR THE WAVE FUNCTION OF THE N -PARTICLE

SYSTEM IN THE MANY-BODY PROBLEM

DALC, 1959, T/26, N 4, C 755-758.

Dubna, 1959

V.G.Soloviev

P.309

EQUATION FOR THE WAVE FUNCTION OF THE N -PARTICLE
SYSTEM IN THE MANY-BODY PROBLEM

$$H \Psi = E \Psi$$

$$H = \sum_{i=1}^N \left(-\frac{\hbar^2}{2m} \nabla_i^2 + V(\mathbf{r}_i) \right) + V(\mathbf{r}_1, \dots, \mathbf{r}_N)$$

$$\Psi(\mathbf{r}_1, \dots, \mathbf{r}_N) = 0$$

$$\Psi(\mathbf{r}_1, \dots, \mathbf{r}_N) = \langle \mathbf{r}_1, \dots, \mathbf{r}_N | \Psi \rangle$$

where $\langle \mathbf{r} | \Psi \rangle = \int \Psi(\mathbf{r}_1, \dots, \mathbf{r}_N) \delta(\mathbf{r}_i - \mathbf{r}) d\mathbf{r}_1 \dots d\mathbf{r}_N$ is the marginal wave function of the i -th particle. In the case of non-stationary processes one should consider the energy E as the eigenvalue corresponding to the time

$$\frac{\partial \Psi}{\partial t} = -\frac{i}{\hbar} H \Psi$$

In the paper ¹ N.N. Bogolubov suggested the new variational principle which is a generalization of the well known Fock method ². The consideration of the new variational principle was extended in ³⁻⁵. In the Fock method the energy minimum is sought among the class of quasi-independent wave functions of the particles while in the new variational principle this energy minimum is sought among wider class of the functions, namely, in addition to the quasi-independent wave functions of the particles one takes into account the wave functions of pairs of particles.

It is well known that in the series of the physical processes the correlations of the several particles play an important part. Indeed, in the phenomenon of superconductivity of electron pairs with equal and opposite momenta near the energy of the Fermi surface play an essential role. In the atomic nucleus the pair correlations of nucleons which are on the outer shell play an important part, and in α -partial model of the nucleus the correlations of the four particles are considered: two protons and two neutrons etc.

In this connection it is interesting to obtain equations which would take into account not only the correlations of two particles but also the correlations of any number of particles. The method suggested by N.N. Bogolubov ⁶ makes it possible to take into account N -particle correlations in the problem where the total number of particles $N' \gg N$, i.e., essentially, to take into account N -particle correlations in the medium. In the present paper we use this method for obtaining an equation for the wave function of the N -particle system in the many body problem, taking into consideration its application to the processes in which the correlations of many particles play an important part.

Let us consider a system of the Fermi-particles interacting with a Hamiltonian:

$$H = \sum_{f, f'} T(f, f') a_f^+ a_{f'} + \frac{1}{2} \sum_{f_1, f_2, f_1', f_2'} K(f_1, f_2, f_1', f_2') a_{f_1}^+ a_{f_2}^+ a_{f_1'} a_{f_2'} \quad (1)$$

where $T(f, f') = E(f, f') - \lambda \delta(f - f')$, the other notations are given in ⁵. In ⁵ using the new variational principle one has obtained equations

$$\mathcal{L}(f, f' | F, \Psi) = 0, \quad \mathcal{B}(f, f' | F, \Psi) = 0 \quad (2)$$

for the functions

$$F(f, f') = \langle a_f^+ a_{f'} \rangle, \quad \Psi(f, f') = \langle a_f a_{f'} \rangle \quad (3)$$

where $\langle A \rangle = \text{Sp} \{ A \mathcal{D} \} / \text{Sp} \mathcal{D}$, i.e. $\langle \dots \rangle$ is the averaging over some statistical operator \mathcal{D} . In the case of non-stationary processes one should consider the amplitudes a_f in Heisenberg representation and then

$$i \frac{\partial F(f, f')}{\partial t} = \langle [a_f^+ a_{f'}, H] \rangle, \quad i \frac{\partial \Psi(f, f')}{\partial t} = \langle [a_f a_{f'}, H] \rangle \quad (4)$$

or, basing on ⁶

$$i \frac{\partial F(f_1, f_2)}{\partial t} = \langle [a_{f_1}^+ a_{f_2}, H] \rangle = \mathcal{B}(f_1, f_2 | F, \phi), \quad i \frac{\partial \Psi(f_1, f_2)}{\partial t} = \mathcal{U}(f_1, f_2 | F, \phi). \quad (5)$$

Let us consider the correlation function

$$\langle a_{x_1} \dots a_{x_N} a_{x'_1}^+ \dots a_{x'_N}^+ \rangle$$

in λ -representation in the case when the number of particles N is a good quantum one; therefore we exclude from (1) the chemical potential λ . Let this correlation function be represented in the form:

$$\langle a_{x_1} \dots a_{x_N} a_{x'_1}^+ \dots a_{x'_N}^+ \rangle = \Psi(x_1, \dots, x_N) \Psi^*(x'_1, \dots, x'_N) + \mathcal{J}, \quad (6)$$

where \mathcal{J} tends rapidly to zero, when the spacing between the systems (x_1, \dots, x_N) and (x'_1, \dots, x'_N) tends to the infinity, and the integrals:

$$\int |\Psi(x_1, \dots, x_N)|^2 dx_i \quad \text{for } 1 \leq i \leq N$$

are convergent ones. In this case one may interpret $\Psi(x_1, \dots, x_N)$ as wave function of the N -particle system.

In order to deduce the equation, which determines $\Psi(x_1, \dots, x_N)$ let us consider the two-time correlation function

$$\langle a_{x_1}(t) \dots a_{x_N}(t) a_{x'_1}^+(\tau) \dots a_{x'_N}^+(\tau) \rangle$$

and differentiate it over the time t ; we obtain:

$$i \frac{\partial}{\partial t} \langle a_{x_1}(t) \dots a_{x_N}(t) a_{x'_1}^+(\tau) \dots a_{x'_N}^+(\tau) \rangle = \quad (7)$$

$$= \langle [a_{x_1}(t) \dots a_{x_N}(t), H] a_{x'_1}^+(\tau) \dots a_{x'_N}^+(\tau) \rangle.$$

This equation contains the correlation functions, including $2N+2$ operators. Let us proceed to the approximate equation expressing approximately the correlation function including $2N+2$ operators in terms of correlation functions of the two and $2N$ operators as follows

$$\langle a_{x_1}^+(t) a_{x_2}(t) \dots a_{x_{j-1}}(t) a_{x_{j+1}}(t) \dots a_{x_N}(t) a_{x'_1}^+(\tau) \dots a_{x'_N}^+(\tau) \rangle = \quad (8)$$

$$= \sum_{\substack{j=1 \\ j \neq i}}^N (-i)^N \langle a_{x_1}^+(t) a_{x_j}(t) \rangle \langle a_{x_2}(t) \dots a_{x_{j-1}}(t) a_{x_{j+1}}(t) \dots a_{x_{i-1}}(t) a_{x_{i+1}}(t) \dots$$

$$\dots a_{x_N}(t) a_{x'_1}^+(\tau) \dots a_{x'_N}^+(\tau) \rangle +$$

$$+ (-1)^{N+1} \langle a_p^\dagger(t) a_p(t) \rangle \langle a_{n_1}(t) \dots a_{n_{r-1}}(t) a_{n_r}(t) \dots a_{n_s}(t) a_{n_s}^\dagger(\tau) \dots a_{n_1}^\dagger(\tau) \rangle +$$

$$+ (-1)^N \langle a_p^\dagger(t) a_p(t) \rangle \langle a_{n_1}(t) \dots a_{n_{r-1}}(t) a_{n_r}(t) \dots a_{n_s}(t) a_{n_s}^\dagger(\tau) \dots a_{n_1}^\dagger(\tau) \rangle + \bar{S}$$

where \bar{S} contains such terms which tend to zero when displacing (x_1, \dots, x_N) to the infinity. Let us note when splitting (8) the number of particles n is conserved. In view of the fact that the wave function ψ_t must be proportional to $e^{-iN\lambda t}$ in the stationary state then in the general non-stationary case we write it as :

$$\psi_t(x_1, \dots, x_N) = e^{-iN\lambda t} \psi(x_1, \dots, x_N) \quad (9)$$

Let us substitute (8) into (7) and displace (x_1, \dots, x_N) to the infinity, then, using (6) we obtain the equation for the wave function of the N - particle system as follows:

$$i \frac{\partial}{\partial t} \psi(x_1, \dots, x_N) + N\lambda \psi(x_1, \dots, x_N) = \sum_{i=1}^N \sum_f E(x_i, f) \psi(x_1, \dots, x_{i-1}, f, x_{i+1}, \dots, x_N) +$$

$$+ \sum_{i>j=1}^N \sum_{f_1, f_2} K(f_1, f_2; x_i, x_j) \psi(x_1, \dots, x_{j-1}, f_1, x_j, f_2, x_{j+1}, \dots, x_{i-1}, f_1, x_{i+1}, \dots, x_N) +$$

$$+ \sum_{i=1}^N \sum_{f, f_1, f_2} \left\{ K(f_1, f_2; x_i, f) F(f, f_1) \psi(x_1, \dots, x_{i-1}, f_1, x_{i+1}, \dots, x_N) + K(f_1, f_2; f, x_i) F(f, f_2) \psi(x_1, \dots, x_{i-1}, f_2, x_{i+1}, \dots, x_N) \right\} -$$

$$- \sum_{i=1}^N \sum_{j=1}^N \sum_{f_1, f_2, f_3} K(f_1, f_2; x_i, f) F(f, f_3) \psi(x_1, \dots, x_{j-1}, f_1, x_j, f_2, x_{j+1}, \dots, x_{i-1}, f_1, x_{i+1}, \dots, x_N).$$

Let us consider the equation for the wave function of the N -particle system in the many-body problem in the two particular cases. The first case $f = (x, \sigma)$

$$E(f, f) = E(x) \delta(f - f) \quad (11)$$

$$K(f_1, f_2; f_1, f_2) = \frac{1}{2} V(f_1, f_2) \left\{ \delta(f_1 - f_2) \delta(f_1 - f_2) - \delta(f_1 - f_2) \delta(f_2 - f_1) \right\},$$

where $V(f_1, f_2) = V(|z_1 - z_2|, \sigma_1, \sigma_2)$. In this case we get the equation (10) in the form:

$$i \frac{\partial}{\partial t} \psi(x_1, \dots, x_N) = \sum_{i=1}^N \left\{ [E(x_i) - \lambda] + \sum_f V(x_i, f) F(f, f) \right\} \psi(x_1, \dots, x_N) -$$

$$- \sum_{i=1}^N \sum_f V(x_i, f) F(f, x_i) \psi(x_1, \dots, x_{i-1}, f, x_{i+1}, \dots, x_N) +$$

$$+ \sum_{i>j=1}^N V(x_i, x_j) \psi(x_1, \dots, x_N) - \sum_{i=1}^N \sum_{j=1, j \neq i}^N V(x_i, f) F(f, x_j) \psi(x_1, \dots, x_{j-1}, f, x_{j+1}, \dots, x_N)$$

and the equation for $F(f, f)$ we write as

(1-F(r)) - F(r) in the interaction term.

In this case the role of the medium is reduced to the appearance of the multiplier

$$F(r) = F(r)^2 + \psi(r)$$

where

$$-F(r) - F(r) \psi(x_1, x_2, \dots, x_n) = 0$$

(15)

$$\sum_{i=1}^n \{ E(r_i) - 1 \} \psi(x_1, \dots, x_n) + \sum_{i=1}^n V(r_i + \dots + r_i) \psi(x_1, \dots, x_n) = 0$$

The equation for $\psi(x_1, \dots, x_n)$ we get in the form:

(16)

$$\psi(r, r) = \psi(r) \delta(r+r) + \psi(r) - \psi(r) = \psi(r)$$

From the Eq. (14) it follows that

(17)

$$F(r, r) = F(r) \delta(r-r)$$

In the representation where F is diagonal, i.e.

(18)

$$V(r_1, r_2, \dots, r_n) = V(r_1, r_2, \dots, r_n) \delta(r_1 + r_2 + \dots + r_n)$$

$$E(r, r) = E(r) \delta(r-r)$$

As the second example we consider the stationary case: $f = (p, \sigma)$

Later one takes into account the correlations of the pairs of particles.

The equation of the Fock method which differs from the equation for $F(r, r)$ by what in the

and when $N = 2$, then (12) coincides with (21) in ψ . In the case when $N = 1$ we obtain

(19)

$$\frac{\partial F(r, r)}{\partial r} = \frac{\partial \psi(x_1, \dots, x_n)}{\partial r} = 0$$

In the stationary case

(20)

$$\sum_{i=1}^n \{ \psi(r_i, r_i) F(r_i, r_i) + \psi(r_i, r_i) F(r_i, r_i) \} = 0$$

$$F(r, r) = \sum_{i=1}^n \{ \psi^*(r_i, r_i) \psi(r_i, r_i) + F(r_i, r_i) F(r_i, r_i) \}$$

where $F(r, r)$ and $\psi(r, r)$ are connected by the relations

(21)

$$+ \sum_{i=1}^n \{ V(r_i, r_i) - V(r_i, r_i) \} \{ F(r_i, r_i) F(r_i, r_i) - F(r_i, r_i) F(r_i, r_i) + \psi^*(r_i, r_i) \psi(r_i, r_i) \}$$

$$\frac{\partial F(r, r)}{\partial r} = \{ E(r) - E(r) \} F(r, r) +$$

Thus, the new variational principle and the mathematical method suggested by N.N.Bogolubov allow to calculate not only pair correlations but also the correlations of N -particles in the many-body problem. Let us note that the number of particles is conserved strictly in the spatially homogeneous problems and is not conserved in the case of the spatially inhomogeneous problems.

In conclusion I express my deep gratitude to the academician N.N.Bogolubov for the increasing interest to the work and highly valuable remarks.

References

1. N.N.Bogolubov, Dokl.Akad.Nauk, 119, 244 (1958).
2. V.A.Fock, Zh.f. Phys. 61, 126 (1930).
3. S.V.Tyablikov, Dokl.Akad.Nauk, 121, 250 (1958).
4. S.V.Tyablikov, Nauchn.Doklady, Vyshey Shkoly 1, n.3 (1956).
5. N.N.Bogolubov, V.G.Soleviev, Dokl.Akad.Nauk, 124, n. 5 (1959).
6. N.N.Bogolubov, UFN 61, n.4 (1959).

The Russian variant of this paper was
received by Publishing Department on February,
23, 1959.