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IN THE MANY BODY PROBLEM

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ON A VARIATIONAL PRINCIPLE IN THE MANY BODY PROBLEM

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БИБЛИОТЕКА

In the paper^{1/} a new variational principle was proposed by one of the authors (N.N.B.). This principle is a generalization of the well known Fock method^{2/}. Consideration of the new variational principle was extended by S.V.Tyablikov^{4,7/}. In this paper we shall make further investigations of the variational principle in the many body problem, obtain stationary equations in a evident form and consider the application of this variational principle to two particular cases.

Let us consider a system interacting Fermi-particles with a Hamiltonian

$$H = \sum_{f,f'} E(f,f') \alpha_f^* \alpha_{f'} + \frac{1}{2} \sum_{f_1, f_2, f'_1, f'_2} K(f'_1, f'_2; f_1, f_2) \alpha_{f_1}^* \alpha_{f_2}^* \alpha_{f'_1} \alpha_{f'_2}, \quad (1)$$

here $E(f,f') = T(f,f') - \lambda \delta_{ff'}$, λ - is the chemical potential, f - set of indices characterising one particle state and the real function $K(f'_1, f'_2; f_1, f_2)$ has the following properties:

$$K(f'_1, f'_2; f_1, f_2) = K(f_2, f_1; f'_1, f'_2) = K(f'_1, f'_2; f_2, f_1) \quad (2)$$

Perform a canonical transformation of the Fermi-amplitudes:

$$\alpha_f = \sum_v \{ U_{fv} d_v + V_{fv} d_v^* \} \quad (3)$$

In order to preserve their commutation properties it is necessary to carry out the following conditions:

$$\Xi_{f,f'} \equiv \sum_v \{ U_{fv} U_{f'v}^* + V_{fv} V_{f'v}^* \} - \delta_{ff'} = 0. \quad (4)$$

$$\Upsilon_{f,f'} \equiv \sum_v \{ U_{fv} V_{f'v} + V_{fv} U_{f'v} \} = 0.$$

We determine a new vacuum state C_0

$$d_v C_0 = 0$$

and find a mean value of H by this state, e.i.

$$\bar{H} = \sum_{f,f'} E(f,f') F(f,f') + \sum_{f_1, f_2, f'_1, f'_2} K(f'_1, f'_2; f_1, f_2) \left\{ F(f,f') F(f'_1, f'_2) + \frac{1}{2} \phi(f,f') \phi(f'_1, f'_2) \right\}, \quad (5)$$

where

$$F(f,f') = \sum_v U_{fv}^* V_{f'v}; \quad \phi(f,f') = \sum_v U_{fv} V_{f'v}. \quad (6)$$

Let us determine U and V from the minimum \bar{H} condition with the subsidiary conditions (4):

$$\delta \left\{ \bar{H}(u,v) + \sum_{f_1, f_2} [\lambda(f_1, f_2) \Xi_{f_1, f_2} + \mu^*(f_1, f_2) \Upsilon_{f_1, f_2} + \mu(f_2, f_1) \Upsilon_{f_1, f_2}^*] \right\} \quad (7)$$

here $\lambda(f,f')$, $\mu(f,f')$ are Lagrange factors. Considering the variations of δu , δv , δu^* , δv^* as independent ones we find:

$$\begin{aligned} \frac{\delta \bar{H}}{\delta U_{f\omega}^*} + \sum_{f''} \left\{ \lambda(f, f'') U_{f\omega} + \mu(f, f'') V_{f\omega}^* + \mu(f'', f) V_{f\omega}^* \right\} &= 0 \\ \frac{\delta \bar{H}}{\delta V_{f\omega}^*} + \sum_{f''} \left\{ \lambda(f, f'') V_{f\omega} + \mu(f, f'') U_{f\omega}^* + \mu(f'', f) U_{f\omega}^* \right\} &= 0 \end{aligned} \quad (8)$$

and two equations complexly conjugated with these. We obtain:

$$\begin{aligned} A(f, f') &= \sum_{\omega} \left\{ U_{f\omega} \frac{\delta \bar{H}}{\delta U_{f\omega}^*} + U_{f\omega} \frac{\delta \bar{H}}{\delta U_{f\omega}^*} \right\} + \mu(f, f') + \mu(f', f) = 0, \\ B(f, f') &= \sum_{\omega} \left\{ U_{f\omega}^* \frac{\delta \bar{H}}{\delta U_{f\omega}^*} + U_{f\omega}^* \frac{\delta \bar{H}}{\delta U_{f\omega}^*} \right\} + \lambda(f, f') = 0. \end{aligned} \quad (9)$$

Let us exclude the Lagrange factors and find the equations:

$$2U(f, f') = A(f, f') - A(f', f) = 0, \quad (10)$$

$$B(f, f') = B(f, f') - B^*(f', f) = 0,$$

which have the following form:

$$2U(f, f') = \sum_{f''} \left\{ \phi(f, f'') \xi(f'', f') - \xi(f, f'') \phi(f'', f') - \right. \quad (11)$$

$$\left. - \sum_{f_1, f_2, f} \left\{ K(f_2, f_1; f, f'') \phi(f, f_2) F(f'', f') - K(f_2, f_1; f', f'') \phi(f, f_2) F(f'', f') \right\} + \right.$$

$$\left. + \sum_{f_1, f_2} K(f_2, f_1; f, f') \phi(f, f_2) = 0, \right.$$

$$B(f, f') = \sum_{f''} \left\{ F(f, f'') \xi(f'', f') - \xi(f, f'') F(f'', f') \right\} + \quad (12)$$

$$+ \sum_{f_1, f_2, f''} \left\{ K(f_2, f_1; f', f'') \phi(f, f_2) \phi^*(f, f'') - K(f_2, f_1; f, f'') \phi^*(f, f_2) \phi(f', f'') \right\} = 0.$$

where

$$\xi(f, f') = E(f, f') + 2 \sum_{f_1, f_2} K(f_2, f; f', f_1) F(f, f_2).$$

(11) and (12) coincide with the equations obtained in [3, 4].

It should be noted that the functions $2U(f, f')$ and $B(f, f')$ are connected by the following relation:

$$\begin{aligned} &\sum_{f, f'} \left\{ U_{f\omega}^* U_{f'\omega}^* 2U(f, f') + U_{f\omega} U_{f'\omega}^* 2U^*(f', f) \right\} + \\ &+ \sum_{f, f'} \left\{ U_{f\omega} U_{f'\omega}^* - U_{f\omega}^* U_{f'\omega} \right\} B(f, f') = 0. \end{aligned} \quad (14)$$

Therefore, if $2U(f, f') = 0$ then it follows from (14) that $B(f, f') = 0$ and one may consider only one of the equations (11), (12). As it was shown in the paper [3] the functions $F(f, f')$ and $\phi(f, f')$ are connected by the following means:

$$\begin{aligned} F(f, f') &= \sum_{f''} \left\{ \phi^*(f'', f) \phi(f'', f') + F(f, f'') F(f'', f') \right\}, \\ &\sum_{f''} \left\{ \phi(f, f'') F(f', f'') + \phi(f', f'') F(f'', f') \right\} = 0. \end{aligned} \quad (15)$$

One may proof these relations by a direct substitution of the expressions $\phi(f, f')$ and $F(f, f')$, if to take the conditions (4) and those connected with them:

$$\sum_f \left\{ U_{f\omega}^* U_{f\omega} + U_{f\omega}^* U_{f\omega} \right\} = \delta_{\omega\omega}, \quad (16)$$

$$\sum_f \left\{ U_{f\omega}^* U_{f\nu} + U_{f\nu}^* U_{f\omega} \right\} = 0.$$

Thus, one may operate with the functions F and ϕ instead of the functions U and ξ , if the conditions (15) carry out, then F and ϕ will be expressed in terms of U and ξ by (6).

We shall consider an application of the new variational principle in the many body problem to two particular cases.

First case. Let us choose $U_{f,v} = U_f \delta(f-v)$, $U_{f,v} = U_f \delta(f+v)$, $U_f = U_f$, $U_f = -U_f$, then $\alpha_f = U_f \alpha_{-f} + U_f \alpha_f^*$, $F(f, f') = \delta(f-f') U_f^2$, $\phi(f, f') = -\delta(f+f') U_f U_{f'}$.

In this case the equation (11) obtains the form:

$$\sum_{f>0} (f, f) U_f U_f + (U_f^2 - U_f^2) \sum_{f>0} K(-f, f'; f, -f) U_{f'} U_{f'} = 0, \quad (18)$$

$$\sum_{f>0} (f, f) = E(f, f) - 2 \sum_{f>0} \{K(f, f; f', f) + K(-f, f; -f', f)\} U_{f'}^2. \quad (19)$$

If $f = (\kappa, \sigma)$, where K is a momentum and σ is a spin, then (18) coincides with an equation of the compensation of "dangerous" graphs in the theory of superconductivity^{5/} and if f is quantum number of the momentum projection along the symmetry axis of the nucleus, then (18) transforms into an equation^{6/}, taking into account an interaction of nucleons, locating on the outer shell of a heavy nucleus.

Second case. Choose $f = (z, \sigma)$ where z - radius-vector, and let us give functions

$K(z'_1, z'_2; z_1, z_2)$, $E(z, z')$ in the form:

$$\frac{1}{2} U(z, -z_2; \sigma_1, \sigma_2) \left\{ \delta_{\sigma_1 \sigma'_1} \delta_{\sigma_2 \sigma'_2}, \delta(z, -z_1) \delta(z_2 - z_2) - \delta_{\sigma_1 \sigma'_1} \delta_{\sigma_2 \sigma'_2}, \delta(z, -z_2) \delta(z_2 - z'_1) \right\},$$

$$E(z) \delta_{\sigma \sigma'}, \delta(z - z') = \{T(z) - h\} \delta_{\sigma \sigma'} \delta(z - z').$$

In this case

$$\begin{aligned} \tilde{H} = & \sum_{z, \sigma} \{T(z) - h\} F(z, \sigma; z, \sigma) + \\ & + \frac{1}{2} \sum_{z_1, \sigma_1, z_2, \sigma_2} U(z, -z_2; \sigma_1, \sigma_2) \left\{ F(z_1, \sigma_1; z_1, \sigma_1) F(z_2, \sigma_2; z_2, \sigma_2) - \right. \\ & \left. - F(z_1, \sigma_1; z_2, \sigma_2) F(z_2, \sigma_2; z_1, \sigma_1) + \phi(z_1, \sigma_1; z_2, \sigma_2) \phi(z_1, \sigma_1; z_2, \sigma_2) \right\} \end{aligned} \quad (20)$$

and the equation (11) will be :

$$\begin{aligned} & \left\{ E(z_1) + E(z_2) + \sum_{z', \sigma'} U(z, -z'; \sigma, \sigma') F(z, \sigma'; z', \sigma') + \right. \\ & \left. + \sum_{z', \sigma'} U(z_2, -z'; \sigma_2, \sigma') F(z', \sigma'; z', \sigma') + U(z, -z_2; \sigma_1, \sigma_2) \right\} \phi(z_1, \sigma_1; z_2, \sigma_2) + \\ & + \sum_{z', \sigma'} \left\{ U(z, -z'; \sigma, \sigma') F(z', \sigma'; z_1, \sigma_1) \phi(z_2, \sigma_2; z', \sigma') + U(z_2, -z'; \sigma_2, \sigma') F(z', \sigma'; z_2, \sigma_2) \right. \\ & \left. + \phi(z', \sigma'; z_1, \sigma_1) \right\} - \sum_{z', \sigma'} \left\{ U(z, -z'; \sigma, \sigma') F(z', \sigma'; z_2, \sigma_2) \phi(z', \sigma'; z_1, \sigma_1) + \right. \\ & \left. + U(z_2, -z'; \sigma_2, \sigma') F(z', \sigma'; z_1, \sigma_1) \phi(z_2, \sigma_2; z', \sigma') \right\} = 0, \end{aligned} \quad (21)$$

Let us write it in the form:

$$\left\{ E_1 + E_2 + V_i + V_2 \right\} \phi_{12} + \sum_K \left\{ E_{ik} \phi_{ik} + E_{2k} \phi_{2k} \right\} + Z_{12} - \sum_K \left\{ Z_{2k} F_{ki} + Z_{ki} F_{k2} \right\} = 0. \quad (22)$$

Here $V_i = \sum_{z, \sigma} U(z_i - z'; \sigma_i, \sigma') F(z, \sigma; z, \sigma)$ is a potential, created by all particles in the point z_i ,

$E_{ik} = U(z_i - z_k; \sigma_i, \sigma_k) F(z_k, \sigma_k; z_i, \sigma_i)$ is an addition to the kinetic energy of the i -particle; the term:

$Z_{12} = U(z_1 - z_2; \sigma_1, \sigma_2) \phi(z_1, \sigma_1; z_2, \sigma_2)$ describes an interaction of the two particles, and the expression

$- \sum \{Z_{2k} F_{ki} + Z_{ki} F_{k2}\}$ takes into account the influence of the others particles, distributed

with the density $F(z, \sigma; z, \sigma)$.

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