

407

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TO THE THEORY OF ATOMIC NUCLEUS

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ON AN APPLICATION OF THE STATISTICAL VARIATIONAL PRINCIPLE
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The statistical variational principle^[1], which is a generalization of the variational principle suggested by Bogoliubov^[2] enables us to calculate thermodynamic quantities at zero temperature as well as at non-zero one.

In the present paper with the aid of the statistical variation principle the superfluid state of the nucleus at nonzero temperature was investigated: the temperature of the phase transition from the superfluid state into the normal one was obtained, the behaviour of thermodynamic quantities at the temperature close to $\theta \approx 0$ as well as at the temperature close to a critical one $\theta = \theta_0$ was investigated.

Just as in the previous papers of one of the authors^[3,4] basing on the shell model of the nucleus we consider residual interactions of nucleons near the Fermi energy surface, i.e.

$$E_F - \delta \leq E(\mathcal{A}, m) \leq E_F + \Delta.$$

Write the Hamiltonian of the residual nucleon interactions in the form:

$$H = \sum_{\mathcal{A}, m, \rho} \left\{ E(\mathcal{A}, m) - \lambda \right\} a_{\rho m}(\mathcal{A})^{\dagger} a_{\rho m}(\mathcal{A}) + \frac{1}{4} \sum_{\substack{\mathcal{A}_1, \mathcal{A}_2; \mathcal{A}'_1, \mathcal{A}'_2 \\ m_1, m_2, m'_1, m'_2 \\ \rho_1, \rho_2, \rho'_1, \rho'_2 \\ \rho_1 m_1 + \rho_2 m_2 = \rho'_1 m'_1 + \rho'_2 m'_2}} J(\mathcal{A}_1, \mathcal{A}_2; \mathcal{A}'_1, \mathcal{A}'_2 | m_1, m_2; m'_1, m'_2) a_{\rho_1 m_1}(\mathcal{A}_1)^{\dagger} a_{\rho_2 m_2}(\mathcal{A}_2)^{\dagger} a_{\rho'_1 m'_1}(\mathcal{A}'_1) a_{\rho'_2 m'_2}(\mathcal{A}'_2) \quad (1)$$

The chemical potential λ is determined from the condition:

$$\lambda = \sum_{\mathcal{A}, m, \rho} \langle a_{\rho m}(\mathcal{A})^{\dagger} a_{\rho m}(\mathcal{A}) \rangle \quad (2)$$

the notations are the same as in^[4]. Let us perform the canonical transformation

$$a_{\rho m}(\mathcal{A}) = U_m(\mathcal{A}) \alpha_{m, -\rho}(\mathcal{A}) + \rho V_m(\mathcal{A}) \alpha_{m \rho}(\mathcal{A})^{\dagger} \quad (3)$$

under the condition

$$\eta_m(\mathcal{A}) = U_m(\mathcal{A})^2 + V_m^*(\mathcal{A})^2 - 1 = 0 \quad (4)$$

and determine a new vacuum state Ψ_0 :

In order to avoid the transition from an even nucleus to an odd one we examine the excited states of the type:

$$\underline{\Psi}_2 = \alpha_{m+}(\mathcal{A})^{\dagger} \alpha_{m-}(\mathcal{A})^{\dagger} \Psi_0. \quad (5)$$

The Hamiltonian is represented by us in the form:

$$H = \langle H \rangle + H_0 + H_1 \quad (6)$$

where

$$H_0 = \sum_{\mathcal{A}, m, \rho} E_m(\mathcal{A}) \alpha_{m \rho}(\mathcal{A})^{\dagger} \alpha_{m \rho}(\mathcal{A})$$

and

$$E_m(\mathcal{A}) = 2 \left\{ E(\mathcal{A}, m) - \lambda \right\} \left\{ U_m(\mathcal{A})^2 - V_m^*(\mathcal{A})^2 \right\} - 4 \sum_{\mathcal{A}', m'} J(\mathcal{A}, \mathcal{A}' | m, m') \cdot U_m(\mathcal{A}) V_m^*(\mathcal{A}) U_{m'}(\mathcal{A}') V_{m'}^*(\mathcal{A}').$$

Making use of the Bogoliubov's variational theorem we get an upper limit for the thermodynamic potential of nucleus in the following form

$$\begin{aligned} \Psi = & -\theta \sum_{s,m} \ln \left\{ 2 \operatorname{ch} \frac{E_m(s)}{\theta} \right\} + \sum_{s,m} \{ E(s,m) - \lambda \} - \\ & - 2 \sum_{s,s',m,m'} J(s,s'|m,m') \operatorname{th} \frac{E_m(s)}{2\theta} u_m(s) v_m(s) u_{m'}(s') v_{m'}(s') + \\ & + \sum_{s,s',m,m'} J(s,s'|m,m') \operatorname{th} \frac{E_m(s)}{2\theta} \operatorname{th} \frac{E_{m'}(s')}{2\theta} u_m(s) v_m(s) u_{m'}(s') v_{m'}(s'). \end{aligned} \quad (8)$$

From the condition of the thermodynamic potential minimum we obtain equation for the determination of u, v :

$$\begin{aligned} \{ E(s,m) - \lambda \} u_m(s) v_m(s) + \frac{8}{\theta} \frac{u_m(s)^2 v_m(s)^2}{\operatorname{sh} \frac{E_m(s)}{\theta}} \sum_{s',m'} J(s,s'|m,m') v_{m'}(s') u_{m'}(s') v_{m'}(s') + \\ + \frac{4}{\theta} \frac{u_m(s) v_m(s)}{\operatorname{sh} \frac{E_m(s)}{\theta}} \{ u_m(s)^2 - v_m(s)^2 \} \sum_{s',m'} J(s,s'|m,m') u_{m'}(s') v_{m'}(s') \sum_{s'',m''} J(s',s''|m',m'') v_{m''}(s'') u_{m''}(s'') v_{m''}(s'') + \\ + \frac{2}{\theta} \{ u_m(s)^2 - v_m(s)^2 \} \operatorname{ch} \frac{E_m(s)}{2\theta} \sum_{s',m'} J(s,s'|m,m') \frac{u_{m'}(s')^2 v_{m'}(s')^2}{\operatorname{ch}^2 \frac{E_{m'}(s')}{2\theta}} \sum_{s'',m''} J(s',s''|m',m'') v_{m''}(s'') u_{m''}(s'') v_{m''}(s'') + \\ + \frac{u_m(s)^2 - v_m(s)^2}{2} \sum_{s',m'} J(s,s'|m,m') \operatorname{th} \frac{E_{m'}(s')}{2\theta} u_{m'}(s') v_{m'}(s') = 0 \end{aligned} \quad (9)$$

where

$$v_m(s) = \frac{1}{1 + e^{E_m(s)/\theta}}.$$

It is easily seen that (9) assumes a trivial solution corresponding to the normal state, viz.

$$u_m(s) = 1 - \theta_F(s, m), \quad v_m(s) = \theta_F(s, m)$$

where $\theta_F(s, m) = 1$ for $E(s, m) < E_F$ and $\theta_F(s, m) = 0$ for $E(s, m) > E_F$.

Considering the second variation of the thermodynamic potential, as in^[3], we obtain the following equation for finding the phase transition temperature

$$2|E(s,m) - \lambda| \operatorname{ch} \frac{|E(s,m) - E_F|}{\theta_0} \varphi_m(s) + \sum_{s',m'} J(s,s'|m,m') \varphi_{m'}(s') = 0. \quad (10)$$

The phase transition temperature θ_0 is determined from the condition: the equation (10) should have a non-zero solution. Taking into account the smallness of $|E(s, m) - E_F|/\theta_0$ and assuming the approximation^[4]

$$J = \text{const.}, \quad \rho = \text{const.} \quad (11)$$

we get the phase transition temperature θ_0 equal to:

$$\theta_0 = - \frac{J\rho}{2} (\Delta + \delta). \quad (12)$$

This expression differs by a factor 2 from the corresponding expression in^[3]. This is re-

lated to that we have considered the excited states of the type (5). It should be noted that the concept temperature of finite nucleus begins to assume a physical sense under rather strong excitation of the nucleus, i.e. near and above the phase transition temperature.

We find a non-trivial solution for the Eq.(9). This can be done in the two limiting cases: when the temperature is close to zero and when the temperature is close to that of the phase transition. In both cases the Eq. (9) takes the following form:

$$\xi_m(s) U_m(s) V_m(s) + \frac{U_m(s)^2 - V_m(s)^2}{2} \sum_{s', m'} J(s, s' | m, m') \frac{\text{th} \frac{E_m(s')}{2\theta}}{2\theta} U_{m'}(s') V_{m'}(s') = 0 \quad (13)$$

where $\xi_m(s) = E(s, m) - \lambda$

Let us introduce a new function:

$$C_m(s) = \sum_{s', m'} J(s, s' | m, m') \frac{\text{th} \frac{E_m(s')}{2\theta}}{2\theta} U_{m'}(s') V_{m'}(s') \quad (14)$$

and assume

$$U_m(s)^2 = \frac{1}{2} \left\{ 1 + \frac{\xi_m(s)}{C_m(s)^2 + \xi_m(s)^2} \right\}$$

$$V_m(s)^2 = \frac{1}{2} \left\{ 1 - \frac{\xi_m(s)}{C_m(s)^2 + \xi_m(s)^2} \right\}$$

then, from the Eq.(13) we obtain $U_m(s) V_m(s) = - \frac{C_m(s)}{2 \{ C_m(s)^2 + \xi_m(s)^2 \}^{1/2}}$

and the equation for $C_m(s)$ takes the form similar to (12) in [5].

$$C_m(s) = - \frac{1}{2} \sum_{s', m'} J(s, s' | m, m') \frac{\text{th} \frac{E_m(s')}{2\theta}}{2\theta} \frac{C_{m'}(s')}{\{ C_{m'}(s')^2 + \xi_{m'}(s')^2 \}^{1/2}} \quad (15)$$

In the approximation of (11) the Eq. (15) is got in the form:

$$1 = - \frac{J\rho}{2} \int_{E_F - \lambda - \delta}^{E_F - \lambda + \Delta} \frac{\text{th} \frac{E(\xi)}{2\theta}}{\sqrt{C^2 + \xi^2}} d\xi \quad (16)$$

where $E(\xi) = E_m(s)$

$$= \frac{2\xi^2}{\sqrt{C^2 + \xi^2}} - \frac{J\rho C^2}{\sqrt{C^2 + \xi^2}} \int_{E_F - \lambda - \delta}^{E_F - \lambda + \Delta} \frac{d\xi'}{\sqrt{C^2 + \xi'^2}} \quad (17)$$

The Eq.(2) describing the chemical potential in this approximation is written as

$$n = \rho \int_{E_F - \lambda - \delta}^{E_F - \lambda + \Delta} \left\{ 1 - \frac{\xi}{\sqrt{C^2 + \xi^2}} \right\} d\xi \quad (18)$$

and the thermodynamic potential of the system in the following form:

$$\Psi = \rho \int_{E_F - \lambda - \delta}^{E_F - \lambda + \Delta} \left\{ -\theta \ln \left(1 + e^{-\frac{E(\xi)}{\theta}} \right) - \frac{E(\xi)}{2} + \xi + \sqrt{\frac{C^2}{C_0^2 + \xi^2}} \right\} d\xi + \frac{C^2}{J}$$

(19)

Note that for $\theta = 0$ the eqs. (16), (18) are solved in a simple manner and the magnitudes of C_0 and λ_0 are obtained in¹⁴.

We find an explicit form of C and λ for each limiting case.

Case I: $\theta \approx 0$ i.e. the temperature θ is close to zero. Expanding

$$\frac{E(\xi)}{2\theta} \approx 1 - e^{-\frac{2\sqrt{C_0^2 + \xi^2}}{\theta}}$$

We obtain

$$1 = -\frac{JP}{2} \int_{E_F - \lambda - \delta}^{E_F - \lambda + \Delta} \frac{d\xi}{\sqrt{C_0^2 + \xi^2}} - K(\theta)$$

where

$$K(\theta) = -\frac{JP}{2} \int_{E_F - \lambda_0 - \delta}^{E_F - \lambda_0 + \Delta} \frac{e^{-\frac{2\sqrt{C_0^2 + \xi^2}}{\theta}}}{\sqrt{C_0^2 + \xi^2}} d\xi$$

Solving (16), (18) in this approximation we get

$$C = \frac{(2\Omega - n)n}{\rho(e^{2/\mathcal{G}} - 1)} e^{1/\mathcal{G}} \left\{ 1 - \frac{K(\theta)}{\mathcal{G}} \operatorname{cth} \frac{2}{\mathcal{G}} \right\} \quad (20)$$

$$E_F - \lambda = \frac{\Omega - n}{\rho(e^{2/\mathcal{G}} - 1)} \left\{ 1 - 2 \frac{K(\theta)}{\mathcal{G}} \frac{1}{1 - e^{-2/\mathcal{G}}} \right\} \quad (21)$$

where $\mathcal{G} = -JP$, n - is the number of nucleons and Ω - is the number of levels near the Fermi surface.

Case II: $\theta \approx \theta_0$ i.e. temperature θ is somewhat less than the phase transition temperature θ_0 .

In this case (13) takes the form:

$$\hat{\xi}_m(s) U_m(s) V_m(s) + \frac{1}{4\theta} \{ U_m(s)^2 - V_m(s)^2 \} \sum_{s', m'} J(s, s' | m, m') U_m(s) V_m(s) = 0 \quad (22)$$

$$C_m(s) = \frac{1}{2\theta} \sum_{s', m'} J(s, s' | m, m') E_m(s) U_m(s) V_m(s)$$

In the approximation of (11) for determining C we obtain the equation

$$1 = \frac{\mathcal{G}}{2\theta} \int_{E_F - \lambda - \delta}^{E_F - \lambda + \Delta} \frac{\xi^2}{C_0^2 + \xi^2} d\xi \quad (23)$$

from where

$$\left(\frac{\partial c^2}{\partial \theta}\right)_{\theta=\theta_0} = -\frac{1}{4\theta_0} \frac{n(2\Omega - n)}{\rho^2}$$

Remaining only the linear term in the expression $c(\theta)$ near $\theta = \theta_0$ we obtain

$$c^2 = \frac{1}{4\rho^2} n(2\Omega - n) \cdot \left(1 - \frac{\theta}{\theta_0}\right)$$

The entropy S and the free energy F of the system are connected with the thermodynamical potential Ψ by the following relations:

$$S = -\frac{\partial \Psi}{\partial \theta} - \frac{d\Psi}{dc^2} \frac{\partial c^2}{\partial \theta}$$

$$F = \theta S + \Psi$$

It is easy to show that the derivative $\frac{d\Psi}{dc^2}$ vanishes in the point θ_0 and owing to this fact the entropy S suffers no jump in the point θ_0 , therefore the phase transition of the system from the superfluid state into the normal one is a phase transition of the second kind.

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455/6