APPLICATION OF THE VARIATIONAL PRINCIPLE IN A NEW METHOD OF THE THEORY OF SUPERCONDUCTIVITY

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APPLICATION OF THE VARIATIONAL PRINCIPLE IN A NEW METHOD OF THE THEORY OF SUPERCONDUCTIVITY

(Presented by Academician N. N. Bogolyubov on 18 XI 1957)

In the work on a new method in the theory of superconductivity ([1]), N. N. Bogolyubov, considering Bardeen' s model ([2]), in order to sum a special class of diagrams constructs the Hamiltonian of an equivalent model dynamical system, which after certain transformations is written in the form (see ([1]), (13))

$$\begin{aligned} H = &\sum_k 2\xi(k)v_k^2 - \frac{J}{V}\sum_{k_1,k_2}\theta(k_1)\theta(k_2)u_{k_1}u_{k_2}v_{k_1}v_{k_2} + \sum_k 2E_e(k)\beta_k^+\beta_k \\ &- \frac{J}{V}\sum_{(k_1\neq k_2)}\left(u_{k_1}^2\beta_{k_1}^+ - v_{k_1}^2\beta_{k_1} - 2u_{k_1}v_{k_1}\beta_{k_1}^+\beta_{k_1}\right)\times \\ &\times\left(u_{k_2}^2\beta_{k_2} - v_{k_2}^2\beta_{k_2}^+ - 2u_{k_2}v_{k_2}\beta_{k_2}^+\beta_{k_2}\right)\theta(k_1)\theta(k_2), \end{aligned} \tag{1}$$

where u_k and v_k are determined by the expressions ([3])

$$u_k^2 = 1 - v_k^2 = \frac{1}{2}\left\{1 + \frac{\xi(k)}{E_e(k)}\right\}, \tag{2}$$

where

$$\xi(k) = E(k) - E(k_F), \qquad E_e(k) = \sqrt{\xi^2(k) + \theta(k)c^2},$$

$$c = 2\omega\exp\left\{-\frac{1}{\rho}\right\}, \qquad \rho = \frac{J}{2\pi^2}\left(k^2\frac{dk}{dE(k)}\right)_{k=k_F},$$

$$\theta(k) = \begin{cases} 1, & |\xi(k)| < \omega, \\ 0, & |\xi(k)| > \omega. \end{cases}$$

J and ω are parameters of the Bardeen model, which, according to ([3]), correspond to the quantities g^2 and $\tilde{\omega}/2$ of the Fröhlich system.

As was shown earlier ([4]), proceeding from the variational principle of N. N. Bogolyubov, one can obtain the basic equations of the phenomenological theories of Weiss and Bragg–Williams; moreover, it turned out that the mathematical apparatus in both cases is extremely similar. Let us apply the method developed in ([4]) to the theory of the phase transition in a superconductor. For this, in (1) we pass from the Pauli amplitudes β_k^+ and β_k to new operators S_k^x, S_k^y, and S_k^z, possessing the properties of ordinary spin operators:

$$\beta_k^+ = S_k^x - iS_k^y; \qquad \beta_k = S_k^x + iS_k^y; \qquad \beta_k^+\beta_k = \frac{1}{2} - S_k^z. \tag{3}$$

When applying the variational principle to such a system, as H_0 we choose a sum of the form

$$H_0 = -\sum_k \mathcal{E}(k)\sigma_k, \tag{4}$$

where $\mathcal{E}(k)$ are as yet undetermined functions, and $\sigma_k = 2S_k^z = \pm 1$ are the usual Ising symbols. Since the contributions from the terms of the Hamiltonian that include S^x or S^y, when the variational principle is applied with such an H_0, are equal to zero, then, discarding them at once, we shall have an equivalent Hamiltonian of the system, similar to the Ising Hamiltonian:

$$H' = U - \sum_k E'(k)\sigma_k - \frac{1}{V}\sum_{(k_1\neq k_2)} F(k_1,k_2)\sigma_{k_1}\sigma_{k_2}, \tag{5}$$

where

$$U = \sum_k \xi(k), \qquad E'(k) = E_e(k) - \frac{2J}{V}u_k v_k \theta(k) \sum_{\substack{k' \\ (k'\neq k)}} u_{k'} v_{k'} \theta(k'), \tag{6}$$

$$F(k_1,k_2) = J u_{k_1} u_{k_2} v_{k_1} v_{k_2} \theta(k_1)\theta(k_2).$$

According to the variational principle, the upper bound of the free energy of the system F has the form

$$F \le F_{\text{sup}} = -\theta \ln \operatorname{Sp}\{e^{-H_0/\theta}\} + \operatorname{Sp}\{(H' - H_0)e^{-H_0/\theta}\}/\operatorname{Sp}\{e^{-H_0/\theta}\}. \tag{7}$$

As in (4), we shall regard the upper bound of its free energy as its approximate value. In calculating the free energy (7) it is necessary to take into account that the operators β^+ and β in (1) correspond to the creation and annihilation of pairs of particles; therefore we shall have

$$F \leq U - 2\theta \sum_k \ln 2 \text{ ch} \frac{\mathcal{E}(k)}{2} - \sum_k (E'(k) - \mathcal{E}(k)) \text{ th} \frac{\mathcal{E}(k)}{2\theta} -$$

$$- \frac{1}{V} \sum_{(k_1 \neq k_2)} F(k_1, k_2) \text{ th} \frac{\mathcal{E}(k_1)}{2\theta} \text{ th} \frac{\mathcal{E}(k_2)}{2\theta}. \tag{8}$$

Determining the functions $\mathcal{E}(k)$ from the condition of a minimum of the upper bound of the free energy, we obtain a system of transcendental equations:

$$\mathcal{E}(k) = E'(k) + \frac{2}{V} \sum_{\substack{k' \\ (k' \neq k)}} F(k, k') \text{ th} \frac{\mathcal{E}(k')}{2\theta}. \tag{9}$$

The solution of these equations, taking into account the concrete form of $F(k, k')$ (6), can be written at once:

$$\mathcal{E}(k) = \frac{\xi^2(k) + \theta(k) c\, \mathcal{E}(k_F)}{\sqrt{\xi^2(k) + \theta(k) c^2}}, \tag{10}$$

where the quantity $\mathcal{E}(k_F)$ is determined by the equation:

$$\frac{\mathcal{E}(k_F)}{c} = \frac{J}{4\pi^2} \int_{k_F - \Delta}^{k_F + \Delta} \frac{k^2\, dk}{\sqrt{\xi^2(k) + c^2}} \text{ th} \left\{ \frac{\xi^2(k) + c\mathcal{E}(k_F)}{2\theta \sqrt{\xi^2(k) + c^2}} \right\}. \tag{11}$$

Let us note that at $\theta = 0$, $\mathcal{E}(k_F) = c$, and we obtain the natural result $\mathcal{E}(k) = E_e(k)$.

Noting that the first factor in the integrand has, for small c, a sharp maximum at the point $k = k_F$, and taking the value of the tangent at this point outside the integral sign, we obtain the approximate equation for $\mathcal{E}(k_F)$:

$$\frac{\mathcal{E}(k_F)}{c} = \text{th} \frac{\mathcal{E}(k_F)}{2\theta}. \tag{12}$$

From it, in particular, it follows that the temperature $\theta_0 = {}^1/_2 c$ is critical, since for $\theta > \theta_0$ we have $\mathcal{E}(k_F) = 0$. However, just in the region $\theta \sim \theta_0$, equation (12) gives only a qualitative approximation to (11), and therefore the values of θ_0 and of the heat capacity in this temperature region are only indicative.

Let us investigate the behavior of the specific heat of the system:

$$C = \frac{1}{2N} \sum_k \mathcal{E}(k) \text{ ch}^{-2} \frac{\mathcal{E}(k)}{2\theta} \cdot \left\{ \frac{\mathcal{E}(k)}{\theta^2} - \frac{1}{\theta} \frac{\partial \mathcal{E}(k)}{\partial \theta} \right\}. \tag{13}$$

At temperatures above the critical temperature, but still sufficiently low, after straightforward calculations we obtain

$$C \simeq \frac{Vmk_F\theta}{3N}, \tag{14}$$

which, naturally, coincides with the heat capacity of a free electron gas at low temperatures.

In the range of temperatures below the critical one, but such that $\theta_0 - \theta \ll \theta_0$, the heat capacity, according to (12) and (13), has a singularity. Indeed, near θ_0

$$\frac{\partial \mathcal{E}(k_F)}{\partial \theta} \simeq -\sqrt{\frac{3\theta_0}{\theta_0 - \theta}},$$

and in the immediate vicinity of the critical point, to within constant terms, we shall have

$$C \simeq \sqrt{\frac{3\theta_0}{\theta_0 - \theta}}\,\frac{Vmk_F\theta_0}{2\pi^2 N}. \tag{15}$$

At very low temperatures, such that $\theta \ll \theta_0$, the heat capacity falls according to an exponential law:

$$C \simeq \frac{Vmk_F c^2\sqrt{2\pi c\theta}}{N\pi^2\theta^2} e^{-c/\theta}. \tag{16}$$

To study the dependence of the entropy on temperature, it is convenient to use the relation

$$\frac{\partial S}{\partial \theta} = \frac{1}{\theta} C. \tag{17}$$

At temperatures above the critical temperature, the entropy increases with increasing temperature according to the law (14). As the temperature is lowered, the entropy curve has a sharp downward kink at the point θ_0 and tends exponentially to zero as $\theta \to 0$.

While writing the present note, the author became aware of the work ([5]), in which the same problem is solved in a more correct manner. The results given above are quite close to the results of ([5]). In particular, the basic equation (11), upon replacing the quantities c entering it by $\mathcal{E}(k_F)$, becomes equation (12) of work ([5]). Therefore, in contrast to ([5]), near the critical temperature our $\mathcal{E}(k_F)$ has, according to (11), a certain smearing.

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