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Abstract

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APPLICATION OF THE VARIATIONAL PRINCIPLE IN THE THEORY OF SUPERCONDUCTIVITY

(Presented by Academician N. N. Bogolyubov, November 30, 1957)

In a preceding note ([1]), by means of the variational principle, the thermodynamic properties of a superconducting system were investigated on the basis of N. N. Bogolyubov' s new method in the theory of superconductivity ([2]). As it turned out, the results thereby obtained gave a good idea of the asymptotically exact (for $V \to \infty$, $N \to \infty$, N/v = const) solution of the problem under consideration ([3]).

In the present work we apply the variational principle to a system whose Hamiltonian H has a more general form than that considered in ([3]):

$$H-\lambda N = \sum_{ks}(E(k)-\lambda)a^+_{k,s}a_{k,s} - \frac{1}{V}\sum_{k\neq k'} J(k,k')a^+_{-k,-1/2}a^+_{k,1/2}a_{k',1/2}a_{-k',-1/2} + H',$$

$$H' = -\frac{1}{V}\sum_{k\neq k',\, q\neq 0} J(k,k',q)a^+_{-k+q,1/2}a^+_{k,1/2}a_{k',1/2}a_{k'+q,-1/2}, \qquad (1)$$

where, in particular,

$$J(k,k') = J\theta(k)\theta(k'), \qquad J(k,k',q) = J\theta(k)\theta(k')\theta(k-q)\theta(k'-q), \qquad (2)$$

$$\theta(k) = \begin{cases} 1, & |\xi(k)| < \omega; \\ 0, & |\xi(k)| > \omega; \end{cases} \qquad \xi(k) = E(k) - \lambda;$$

J and ω are Bardeen parameters, and λ is the chemical potential. In contrast to ([3]), where only the interaction of pairs of electrons with opposite momenta was taken into account, in the Hamiltonian (1) terms with $q \neq 0$ are also considered.

Following the main idea of the works of N. N. Bogolyubov, we pass in (1) to new Fermi operators by performing the canonical transformation

$$a_{k,1/2} = u_k\alpha_{k0} + v_k\alpha^+_{k1}, \qquad a_{-k,-1/2} = u_k\alpha_{k1} - v_k\alpha^+_{k0}, \qquad u_k^2 + v_k^2 = 1. \quad (3)$$

The real functions u_k and v_k have not yet been determined. We obtain:

$$H - \lambda N = U + \sum_k \{A(k)(\alpha^+_{k0}\alpha_{k0} + \alpha^+_{k1}\alpha_{k1}) + B(k)(\alpha^+_{k0}\alpha^+_{k1} + \alpha_{k1}\alpha_{k0})\} -$$

$$-\frac{1}{V}\sum_{k\neq k'} J(k,k')\{u_{kv}k(\alpha^+_{k0}\alpha_{k0} + \alpha^+_{k1}\alpha_{k1}) - u_k^2\alpha_{k1}\alpha_{k0} + v_k^2\alpha^+_{k0}\alpha^+_{k1}\}\times$$

$$\times\{u_{k'}v_{k'}(\alpha^+_{k'0}\alpha_{k'0} + \alpha^+_{k'1}\alpha_{k'1}) - u^2_{k'}\alpha^+_{k'0}\alpha^+_{k'1} + v^2_{k'}\alpha_{k'1}\alpha_{k'0}\} + H', \qquad (4)$$

where

$$U = \sum_k \xi(k)\, 2v_k^2 - \sum_k u_k v_k C(k),$$

$$A(k) = \xi(k)(u_k^2 - v_k^2) + 2u_{kv}kC(k), \qquad B(k) = 2\xi(k)u_{kv}k - (u_k^2 - v_k^2)C(k), \ (5)$$

$$C(k) = \frac{1}{V}\sum_{k'(k'\neq k)} J(k,k')u_{k'}v_{k'}.$$

According to N. N. Bogolyubov' s variational principle ([4]) we have:

$$\Psi = -\theta \ln \mathrm{Sp}\{e^{-(H-\lambda N)/\theta}\} \leq -\theta \ln \mathrm{Sp}\{e^{-H_0/\theta}\} +$$

$$+\mathrm{Sp}\{(H - \lambda N - H_0)e^{-H_0/\theta}\}/\,\mathrm{Sp}\{e^{-H_0/\theta}\}. \qquad (6)$$

As H_0 in (4) we choose a form quadratic in the operators α:

$$H_0 = \sum_k \{A(k)(\alpha^+_{k0}\alpha_{k0} + \alpha^+_{k1}\alpha_{k1}) + B(k)(\alpha^+_{k0}\alpha^+_{k1} + \alpha_{k1}\alpha_{k0})\} + \mathrm{const}, \qquad (7)$$

where the constant term will be chosen below for reasons of convenience. The right-hand side of expression (6) contains the functions u_k and v_k, which play the role of variational parameters; the equations for them can be obtained from the requirement that the upper bound of Ψ be minimal. To calculate expression (6) it is convenient to pass to a representation in which H_0 is diagonal. It is not difficult to see that for this purpose one must use the transformation

$$\alpha_{k0} = \lambda_k \beta_{k0} - \mu_k \beta_{k1}^+, \qquad \alpha_{k1} = \lambda_k \beta_{k1} + \mu_k \beta_{k0}^+, \qquad \lambda_k^2 + \mu_k^2 = 1, \tag{8}$$

where λ_k and μ_k are rather complicated functions of u_k and v_k:

$$\lambda_k^2 = 1 - \mu_k^2 = \frac{1}{2}\left(1 + \frac{A(k)}{\sqrt{A^2(k) + B^2(k)}}\right). \tag{9}$$

We shall take into account that the terms nondiagonal in the amplitudes β in the expression $H - \lambda N - H_0$, appearing in the second term of (6), will be equal to zero after the operation Sp; therefore, in the twice-transformed Hamiltonian (1) such terms will be omitted, and in what follows we shall consider the effective Hamiltonian thus obtained. It is easy to see that, in this case, the contribution from the sum H' will also be zero. The expression for the effective Hamiltonian will be simplified still further if, from the occupation numbers $\beta^+\beta = 0$; 1, we pass to the Ising symbols $\sigma = \pm 1$:

$$\beta_{k0}^+ \beta_{k0} + \beta_{k1}^+ \beta_{k1} - 1 = -\frac{\sigma_{k0} + \sigma_{k1}}{2}. \tag{10}$$

Then

$$H_{\text{eff}} = \sum_k \xi(k) - \sum_k \sqrt{\xi^2(k) + C^2(k)}\,\frac{\sigma_{k0} + \sigma_{k1}}{2} + \sum_k \frac{C^2(k)}{\sqrt{\xi^2(k) + C^2(k)}}\,\frac{\sigma_{k0} + \sigma_{k1}}{2} -$$

$$- \frac{1}{4V} \sum_{k \neq k'} J(k, k')\, \frac{C(k)}{\sqrt{\xi^2(k) + C^2(k)}}\, \frac{C(k')}{\sqrt{\xi^2(k') + C^2(k')}}\, \frac{\sigma_{k0} + \sigma_{k1}}{2}\, \frac{\sigma_{k'0} + \sigma_{k'1}}{2}, \tag{11}$$

where, according to (7), H_0 has the form:

$$H_0 = -\sum_k \sqrt{\xi^2(k) + C^2(k)}\,\frac{\sigma_{k0} + \sigma_{k1}}{2}. \tag{12}$$

It is interesting to note that in this form of writing the Hamiltonian the variational functions u_k and v_k enter only in the form of the combination $C(k)$. For the potential Ψ, which is taken to be equal to the right-hand side of (6), we obtain

$$
\begin{aligned}
\Psi = & -2\theta \sum_k \ln 2\,\mathrm{ch}\, \frac{\sqrt{\xi^2(k) + C^2(k)}}{2\theta} + \sum_k \xi(k) \\
& + \sum_k \frac{C^2(k)}{\sqrt{\xi^2(k) + C^2(k)}}\, \mathrm{th}\, \frac{\sqrt{\xi^2(k) + C^2(k)}}{2\theta} \\
& - \frac{1}{4V} \sum_{k \neq k'} J(k, k')\, \frac{C(k)}{\sqrt{\xi^2(k) + C^2(k)}} \times \\
& \quad \times \frac{C(k')}{\sqrt{\xi^2(k') + C^2(k')}}\, \mathrm{th}\, \frac{\sqrt{\xi^2(k) + C^2(k)}}{2\theta}\, \mathrm{th}\, \frac{\sqrt{\xi^2(k') + C^2(k')}}{2\theta}.
\end{aligned}
\tag{13}
$$

Minimizing this expression with respect to $C(k)$, we shall have the equation:

$$
C(k) = \frac{1}{2V} \sum_{k'} J(k, k')\, \frac{C(k')}{\sqrt{\xi^2(k') + C^2(k')}}\, \mathrm{th}\, \frac{\sqrt{\xi^2(k') + C^2(k')}}{2\theta}, \tag{14}
$$

whose solution, when substituted into (13), completely determines the thermodynamic potential Ψ.

Thus, in treating the Hamiltonian (1) by the variational method, the interaction part H'' proved to be inessential, whereas the interaction of pairs of particles with opposite momenta and spins is fundamental. In this way we arrived at the results (13) and (14), which are asymptotically exact ([3]) for the simplified model of a superconductor. It should be emphasized that the results obtained are a consequence of the specific choice of H_0 according to (7).

An analogous situation occurred in the consideration of the Heisenberg and Ising models of a ferromagnet, where, for the simplest choice of H_0, the variational principle led in both cases to identical results.

In note ([1]) the problem of the thermodynamics of a superconductor was solved by a cruder method; namely, the mixing of the operators (3) was assumed from the very beginning in the form in which it is carried out at $\theta = 0$, while all changes arising in the system with increasing temperature were taken into account by means of the most suitable choice of the zero Hamiltonian. Indeed, if in the Hamiltonian (11) one regards $C(k)$ as independent of temperature, and chooses as H the expression

$$
H_0 = -\sum_k E(k) \frac{\sigma_{k0} + \sigma_{k1}}{2}, \tag{15}
$$

then, carrying out the calculation of the upper bound of the thermodynamic potential in (6) and minimizing it with respect to $E(k)$, we obtain the basic relations of work ([1]).

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