PHYSICS

1963

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Abstract

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PHYSICS

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ON ACCOUNTING FOR THE COULOMB INTERACTION IN THE THERMODYNAMICS OF SUPERCONDUCTIVITY

(Presented by Academician N. N. Bogolyubov on 25 VI 1962)

The thermodynamics of superconductivity developed in works ([1–6]) does not explicitly take into account the Coulomb interaction between electrons. In the present note the influence of this interaction on certain parameters of a superconductor is investigated.

The Hamiltonian of the system is chosen in the form ([7]):

$$H = H_0 + H_i; \tag{1}$$

$$H_0 = \sum_{k\sigma} T(k) a^+_{k\sigma} a_{k\sigma} + \sum_q \omega_q b^+_q b_q + H_b; \tag{2}$$

$$H_i = \sum_\sigma \int dx\, \psi^+(x\sigma)\psi(x\sigma)\Phi(x); \tag{3}$$

$$\Phi(x) = g\varphi(x) + e\chi(x). \tag{4}$$

In (1) the direct interaction of electrons is replaced by an interaction through the quantum field χ ([8]) with free Hamiltonian H_b. The operator χ satisfies the additional condition ([7])

$$D_b(x - x') = \langle T\chi(x)\chi(x')\rangle = -v(\mathbf{x} - \mathbf{x}')\delta(\tau - \tau'), \tag{5}$$

where $\langle ... \rangle$ denotes the statistical average over the states of the Hamiltonian H_0; $e^2 v(x)$ is the Coulomb energy of the electrons; the notation for the remaining quantities in (1) is generally accepted.

On the basis of (4) and (5) we have:

$$D(x - x') = \langle T\Phi(x)\Phi(x')\rangle = D_{\text{ph}}(x - x') - e^2 v(\mathbf{x} - \mathbf{x}')\delta(\tau - \tau'), \tag{6}$$

where $D_{\text{ph}}(x)$ is the phonon Green' s function.

Let us consider the complete one-electron Green' s functions:

$$G_{\sigma\sigma'}(x-x') = \delta_{\sigma\sigma'}G(x-x') = \langle T\psi(x\sigma)\bar{\psi}(x'\sigma')U(\beta)\rangle_c,$$

$$R_{\sigma\sigma'}(x-x') = (-1)^{\sigma+1/2}\delta_{\sigma,-\sigma'}R(x-x') = \langle T\psi(x\sigma)\psi(x'\sigma')U(\beta)\rangle_c, \quad (7)$$

$$P_{\sigma\sigma'}(x-x') = (-1)^{\sigma-1/2}\delta_{\sigma,-\sigma'}P(x-x') = \langle T\bar{\psi}(x\sigma)\bar{\psi}(x'\sigma')U(\beta)\rangle_c,$$

where $U(\beta)$ is the evolution operator of the system; c is an index indicating the connected character of diagrams. The anomalous Green' s functions R and P ($^{9-11}$) are considered, according to N. N. Bogolyubov (^{12}), as quasiaverages. In accordance with this, the Green' s functions and the quantities associated with them are introduced by adding to the Hamiltonian (1) infinitely small terms that violate the conservation law of particle number.

In this way we obtain the Dyson equations ($^{9-11}$)

$$G(x-x') = G^0(x-x') + \int_0^\beta\int_0^\beta dx_1 dx_2\, G^0(x-x_1)[\sigma(x_1-x_2)G(x_2-x') - \Sigma(x_1-x_2)P(x_2-x')],$$

$$P(x-x') = \int_0^\beta\int_0^\beta dx_1 dx_2\, G^0(x_1-x)[\sigma(x_2-x_1)P(x_2-x') + \Xi(x_1-x_2)G(x_2-x')] \quad (8)$$

and an analogous equation for the function R. In (8), σ, Σ, and Ξ are electron mass operators, and G^0 is the zero-order Green' s function.

For the exact boson Green' s function

$$B(x-x') = \langle T\Phi(x)\Phi(x')U(\beta)\rangle_c \quad (9)$$

there is the usual Dyson equation with the polarization operator $\Pi(x)$.

Let us also consider one of the vertex Green's functions and the vertex operators Γ, Δ, Λ associated with them:

$$W(x\sigma, x'\sigma'|y) = \langle T\psi(x\sigma)\bar{\psi}(x'\sigma')\Phi(y)U(\beta)\rangle_c =$$
$$= -\delta_{\sigma\sigma'}\int_0^\beta \cdots \int_0^\beta dx_1 \ldots dx_3 B(y-1)\{G(x-2)[\Gamma(23|1)G(3-x') -$$
$$- \Lambda(23|1)P(3-x')] - R(x-2)[\Delta(23|1)G(3-x') - \Gamma(32|1)P(3-x')]\}. \quad (10)$$

In the expressions given, in addition to the usual sign rule, the factor $(-1)^l$ is taken into account, where l is the number of pairs of anomalous quantities R, P, Σ, etc.

For the mass and polarization operators the Dyson equations hold:

$$\sigma(x-x') = \int_0^\beta \int_0^\beta dx_1\, dx_2\, B(x_2 - x)[G(x-x_1)\Gamma(x_1 x'|x_2) - \\ - R(x-x_1)\Delta(x, x'|x_2)],$$

$$\Sigma(x-x') = \int_0^\beta \int_0^\beta dx_1\, dx_2\, B(x - x_2)[G(x-x_1)\Lambda(x_1 x'|x_2) + \\ + R(x-x_1)\Gamma(x' x_1|x_2)],$$

$$\Pi(x-x') = \int_0^\beta \int_0^\beta dx_1\, dx_2 \{G(x-1)[\Gamma(12|x')G(2-x) - \Lambda(12|x')P(2-x)] - \\ - R(x-2)[\Delta(21|x')G(1-x) + \Gamma(21|x')P(1-x)]\}. \tag{11}$$

At $T = 0^\circ$K and in the absence of Coulomb interaction, the first two equations (11) are contained in the monograph ([13]).

On the basis of these formulas and the definition of the thermodynamic potential

$$\Psi = \Psi_0 - \beta^{-1}\langle U(\beta)\rangle_c \tag{12}$$

by differentiating with respect to the coupling constant λ ($\lambda = 1$) we obtain:

$$\Psi = \Psi_0 - \beta^{-1}\int_0^1 \frac{d\lambda}{\lambda}\int_0^\beta \int_0^\beta dx_1\, dx_2\, \Pi(x_1 - x_2)B(x_2 - x_1) = \\ = \Psi_0 + 2\beta^{-1}\int_0^1 \frac{d\lambda}{\lambda}\int_0^\beta \int_0^\beta dx_1\, dx_2 [\sigma(x_1 - x_2)G(x_2 - x_1) - \Sigma(x_1 - x_2)P(x_2 - x_1)], \tag{13}$$

where Ψ_0 is the thermodynamic potential of free electrons and phonons. In (13) all the integrand functions contain the factor λ at the vertices of the diagrams.

In connection with the transition to the momentum representation, let us note the possibility of replacing, in observable quantities, the δ-function on the right-hand side of (5) by an expression periodic in τ with period β, which permits periodic continuation ([14,15]), along with the electronic Green' s function, also of the boson Green' s function. To carry out approximate calculations we shall use the simplest expression for the vertex operator Γ, while taking Λ and Δ equal to zero.

Under these assumptions, for the operator $\Sigma(k)$ $(k = \mathbf{k}, \Omega_n = (2n+1)\pi\beta^{-1})$ we obtain the Dyson equation:

$$\Sigma(k) = (\beta V)^{-1} \sum_{k_1} B(k-k_1)\Sigma(k_1)A(k_1)^{-1}, \tag{14}$$

$$A(k) = -\left\{ i\Omega_n + \frac{\sigma(k)-\sigma(-k)}{2} \right\}^2 + \left\{ T(k) - \frac{\sigma(k)+\sigma(-k)}{2} \right\}^2 + \Sigma(k)\Sigma(-k).$$

Let us further assume that the quantities σ and Σ in the neighborhood of the zeros of the function A are smooth functions of Ω_n, which makes it possible to write in this region the approximate expression

$$A(k) \approx (\Omega_n - i\Omega_k)(\Omega_n + i\Omega_k),$$

$$\Omega_k = \left\{ \left(T(k) - \frac{\sigma(\mathbf{k} \mid \Omega_k) + \sigma(-\mathbf{k} \mid \Omega_k)}{2} \right)^2 + \Sigma(\mathbf{k} \mid \Omega_k)\Sigma(-\mathbf{k} \mid -\Omega_k) \right\}^{1/2}. \tag{15}$$

In these approximations it proves possible, with asymptotic accuracy in the limiting case of weak interaction (3), to compute the quantity Σ, which according to (15) plays the role of a gap in the spectrum of one-particle excitations. Equation (14) for Σ is thereby a generalization of the well-known Bogoliubov compensation equation. Taking the Coulomb interaction into account at $\beta = \infty$, this equation was studied in papers [16–18]. Introduce the notation:

$$\Sigma(k \mid \Omega_n) = \Sigma(k_F \mid 0)F(\mathbf{k} \mid \Omega_n), \qquad F(k_F \mid 0) = 1,$$

$$\xi(k) = T(k) - \frac{1}{2}\left[\sigma(k \mid \Omega_k) + \sigma(k \mid -\Omega_k)\right],$$

$$F_1(\mathbf{k} \mid \Omega_n) = \frac{1}{2\pi} \oint_C dz\, \frac{1}{V} \sum_{\mathbf{k1}} \frac{B(\mathbf{k}-\mathbf{k}_1 \mid \Omega_n - z)F(\mathbf{k}_1 \mid z)}{(z - i\Omega_{k_1})(z + i\Omega_{k_1})},$$

$$\overline{B}(kk_1 \mid \omega_n) = \frac{1}{4\pi} \int d\Omega\, B(\mathbf{k}-\mathbf{k}_1 \mid \omega_n); \tag{16}$$

C is a contour enclosing only the poles of the function $B(q)$, and after simple transformations we represent equation (14) in the form:

$$F(\mathbf{k} \mid \Omega_n) = \frac{1}{2V} \sum_{k_1} \left\{ \frac{B(\mathbf{k}-\mathbf{k}_1 \mid \Omega_n - i\Omega_{k_1}) F(\mathbf{k}_1 \mid i\Omega_{k_1})}{\Omega_{k_1}\left(1+e^{-\beta\Omega_{k_1}}\right)} - \right.$$

$$\left. - \frac{B(\mathbf{k}-\mathbf{k}_1 \mid \Omega_n - i\Omega_{k_1}) F(\mathbf{k}_1 \mid -i\Omega_{k_1})}{\Omega_{k_1}\left(1+e^{\beta\Omega_{k_1}}\right)} \right\} + F_1(\mathbf{k} \mid \Omega_n). \tag{17}$$

The first term in (17) has a logarithmic singularity on the Fermi surface at $\beta = \infty$ and $\Sigma \to 0$, as well as for $\Sigma = 0$ and $\beta \to \infty$. We shall use the method of extracting this singularity, developed by D. N. Zubarev and Yu. A. Tserkovnikov [19]. In this way we obtain:

$$F(\mathbf{k} \mid \Omega_n) = \sum_{i=1}^{2} F_i(\mathbf{k} \mid \Omega_n) - \frac{k_F^2}{2\pi^2 \xi_F'} \overline{B}(kk_F \mid \Omega_n) \left\{ \ln \Sigma(k_F \mid 0) \left| \operatorname{th} \frac{\beta|\Sigma(k_F \mid 0)|}{2} \right| \right.$$

$$- \ln 2 + \left(1 - \operatorname{th} \frac{\beta|\Sigma(k_F \mid 0)|}{2}\right) \ln \frac{2}{\beta} +$$

$$\left. + \int_{\beta|\Sigma(k_F|0)|/2}^{\infty} dt \, \ln \left[t + \left(t^2 - \beta^2 |\Sigma(k_F \mid 0)|^2/4\right)^{1/2} \right] \operatorname{ch}^{-2} t \right\}, \tag{18}$$

where

$$F_2(\mathbf{k} \mid \Omega_n) = (4\pi^2)^{-1} \int_0^{k_F} \ln(-\xi_{k_1}) \, d \left[\frac{k_1^2}{\xi_{k_1}'} \overline{B}(kk_1 \mid \Omega_n + i\xi_{k_1}) F(\mathbf{k}_1 \mid -i\xi_{k_1}) \right] -$$

$$-(4\pi^2)^{-1} \int_{k_F}^{\infty} \ln \xi_{k_1} \, d \left[\frac{k_1^2}{\xi_{k_1}'} \overline{B}(kk_1 \mid \Omega_n - i\xi_{k_1}) F(\mathbf{k}_1 \mid i\xi_{k_1}) \right]. \tag{19}$$

We note that in the functions F_1 and F_2 we have set $\beta = \infty$ and $\Sigma = 0$. The quantity k_F is determined by the condition $\xi(k_F) = 0$. Let us denote:

$$\tilde{\rho} = \frac{k_F^2}{2\pi^2} (\xi_F')^{-1} \overline{B}(k_F k_F \mid 0), \quad \tilde{\rho} \ln \tilde{\omega} = \sum_{i=1}^{2} F_i(k_F \mid 0). \tag{20}$$

Putting $k = k_F$ and $\Omega_n = 0$ in (18), we obtain the transcendental equation

$$-\frac{1}{\tilde{\rho}} = -\ln\tilde{\omega} + \ln|\Sigma(k_F \mid 0)| \text{ th } \beta|\Sigma(k_F \mid 0)|/2 - \ln 2 +$$

$$+\left(1 - \text{th}\,\frac{\beta|\Sigma(k_F \mid 0)|}{2}\right)\ln\frac{2}{\beta} + \int_{\beta|\Sigma(k_F|0)|/2}^{\infty} dt\,\ln\left[t + \left(t^2 - \beta^2|\Sigma(k_F \mid 0)|^2/4\right)^{1/2}\right]\text{ch}^{-2}\,t \tag{21}$$

for determining $\Sigma(k_F \mid 0)$ as a function of the parameters β and $\tilde{\rho}$. In this case the quantity F is found from the equation

$$F(k \mid \Omega_n) = \sum_{i=1}^{2}\left\{F_i(k \mid \Omega_n) - \frac{\overline{B}(kk_F \mid \Omega_n)}{\overline{B}(k_{Fk}F \mid 0)}F_i(k_F \mid 0)\right\} + \frac{\overline{B}(kk_F \mid \Omega_n)}{\overline{B}(k_{Fk}F \mid 0)}. \tag{22}$$

On the basis of (21), for $\Sigma(k_F \mid 0)$ at absolute-zero temperature ($\beta = \infty$) we obtain

$$\Sigma(k_F \mid 0) = 2\tilde{\omega}\exp(-1/\tilde{\rho}). \tag{23}$$

For the critical temperature ($\Sigma = 0$), from the same equation it follows that

$$\frac{1}{\beta_c} = kT_c = \frac{\tilde{\omega}}{2}\exp\left(-\frac{1}{\tilde{\rho}} - \int_0^{\infty}\frac{\ln t}{\text{ch}^2\,t}\,dt\right) \simeq 1.134\,\tilde{\omega}\exp(-1/\tilde{\rho}). \tag{24}$$

These expressions are analogous to the formulas obtained without taking the Coulomb interaction into account ([2,3]), and are valid for positive and sufficiently small values of the parameter $\tilde{\rho}$.

The author takes this opportunity to express his deep gratitude to Academician N. N. Bogoliubov, D. N. Zubarev, S. V. Tyablikov, and Yu. A. Tserkovnikov for valuable advice and attention to the work.

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Received
20 VI 1962

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