PHYSICS

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1962

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Abstract

Full Text

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CRITERION OF SUPERCONDUCTIVITY

(Presented by Academician N. N. Bogolyubov on 28 V 1962)

Let us consider the normal state of a metal in the Fröhlich model, taking into account the Coulomb interaction between electrons. The ground state of this system is stable if the energies of all elementary excitations are positive. Violation of this condition for certain elementary excitations at definite values of the parameters of the metal indicates the instability of the system with respect to these excitations, whence it follows that either the system must pass into another state, or, if such a transition is impossible, the corresponding values of the parameters are incompatible with the theory under consideration. N. N. Bogolyubov [1], and also D. N. Zubarev [2], noted that the appearance above the principal normal state of the metal of elementary excitations consisting of pairs of particles with opposite momenta and spins and with imaginary energies indicates the instability of the normal state and, consequently, the transition of the metal into the superconducting state.

The purpose of the present work is to clarify the role of the Coulomb interaction of electrons in the process of establishing the superconducting state in metals (while neglecting a number of other important properties of metals). We note that the criterion of superconductivity with allowance for the Coulomb interaction of electrons was also investigated in works [3] on the basis of the equations of the superconducting state.

Passing to the writing of the Hamiltonian of the system H, we note that the direct interaction between electrons is conveniently represented as an interaction through an auxiliary quantum Bose field [4] $\chi(x)$. Then we can write:

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

where

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

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

The notation for the electronic and phonon quantities is standard (see, for example, [1]); H_b is the Hamiltonian of the auxiliary quantum field χ. The operator $\chi(x)$, defined in the interaction representation, is subject to the additional condition

$$D_b(x-x') = -i\langle T\chi(x)\chi(x')\rangle_0 = v(x-x')\delta(t-t'), \tag{4}$$

where the symbol $\langle ... \rangle_0$ here and below denotes averaging over the ground state of the Hamiltonian H_0; $v(x)$ is the potential energy of interaction of the electrons.

Let us consider the exact one-particle Green' s functions:

$$G_{\sigma\sigma'}(x-x') = \delta_{\sigma\sigma'}G(x-x') = -i\langle T\psi(x\sigma)\psi^+(x'\sigma')S\rangle_0/\langle S\rangle_0; \tag{5}$$

$$B(x-x') = -i\langle T\Phi(x)\Phi(x')S\rangle_0/\langle S\rangle_0 \tag{6}$$

and the two-particle electron Green' s function

$$G(x_1\sigma_1x_2\sigma_2;\, x_1'\sigma_1'x_2'\sigma_2') = -\langle T\psi(x_1\sigma_1)\psi(x_2\sigma_2)\psi^+(x_2'\sigma_2')\psi^+(x_1'\sigma_1')S\rangle_0/\langle S\rangle_0, \tag{7}$$

where the S-matrix is equal to

$$S = T\exp\left[-i\int_{-\infty}^{\infty} H_i(t)\,dt\right]. \tag{8}$$

In formulas (5)–(7) all operators are taken in the interaction representation.

The pole of the two-particle Green' s function, which determines the energy of a bound pair of electrons or holes, is found from the solution of the following homogeneous equation ([5,6]):

$$F(x_1x_2;\sigma_1\sigma_2) = \int\cdots\int\sum_{s_1s_2} G(x_1-y_1)G(x_2-y_2)K(y_1\sigma_1y_2\sigma_2;\, y_1's_1y_2's_2)\times$$

$$\times F(y_1'y_2';\, s_1s_2)\,dy_1\ldots dy_2'. \tag{9}$$

For simplicity, in what follows we shall restrict ourselves to an operator K of the form

$$K(y_1\sigma_1y_2\sigma_2;\, y_1's_1y_2's_2) = iB(y_1-y_2)\delta(y_2-y_2')\delta_{\sigma_1s_1}\delta_{\sigma_2s_2}. \tag{10}$$

In this approximation equation (9) takes the form:

$$F(x_1x_2;\sigma_1\sigma_2) = i\iint dy_1dy_2\, G(x_1-y_1)G(x_2-y_2)B(y_1-y_2)F(y_1y_2;\sigma_1\sigma_2). \tag{11}$$

Let us separate in the wave function F the translational motion of the pair of particles:

$$F(x_1x_2;\sigma_1\sigma_2) = \exp[-iP(x_1+x_2)/2]\, f_P(x_1-x_2), \qquad P = (\mathbf{P}, 2\omega), \tag{12}$$

and perform in (11) a Fourier transformation with respect to all quantities; then we obtain:

$$f_P(p') = iG\left(\frac{P}{2}+p'\right)G\left(\frac{P}{2}-p'\right)\int \frac{d^4p_1}{(2\pi)^4}\, B(p'-p_1)f_P(p_1). \tag{13}$$

Let us consider the simplest case, when the total momentum of the pair under consideration $\mathbf{P}$ is equal to zero; then (13) takes the form

$$f_{2\omega}(pp^0) = iG(\omega+p^0 \mid \mathbf{p})G(\omega-p^0 \mid -\mathbf{p})U_\omega(p \mid p^0), \tag{14}$$

where the function U_ω and the corresponding energy 2ω of the bound pair of particles are determined from the equation

$$U_\omega(p \mid p^0) = \tag{15}$$

$$= i\int \frac{dp_1\, dp_1^0}{(2\pi)^4} B(\mathbf{p}-\mathbf{p}_1 \mid p^0-p_1^0)G(p_1^0+\omega \mid \mathbf{p}_1) \times G(\omega-p_1^0 \mid -\mathbf{p}_1)U_\omega(\mathbf{p}_1 \mid p_1^0).$$

The further simplifications necessary for solving this equation consist in retaining only the pole parts of the functions G and B. Using the results of works ([6,7]), near the Fermi surface we have

$$G(p) \simeq Z(p)(p^0 - T(p) + i\gamma(p))^{-1}, \tag{16}$$

where $T(p)$ is the energy of the elementary excitation in the effective-mass approximation ($m_{\text{eff}} \sim m$); $\gamma(p)$ is a small damping; $Z(p) \sim 1$. On the basis of the simplest polarization operator we obtain ([8])

$$B(qq^0) \simeq \tilde{D}_b(q) + \tilde{D}_{ph}(qq^0), \tag{17}$$

where

$$\tilde{D}_b(q) = \frac{2\pi^2 T'_F}{p_F^2}\,\frac{\rho'}{x^2 + \rho'\eta(x)}; \tag{18}$$

$$\tilde{D}_{ph}(qq^0) = -\frac{g_e^2(q)\omega_e(q)}{2}\left(\frac{1}{\omega_e(q) - q^0 - i\delta} + \frac{1}{\omega_e(q) + q^0 - i\delta}\right); \tag{19}$$

$$\omega_e^2(q) = \omega^2(q)\left(x^2 + \eta(x)(\rho' - \rho x^2)\right)\left(x^2 + \rho'\eta(x)\right)^{-1}; \tag{20}$$

$$g_e^2(q)\,\omega_e^2(q) = g^2\omega^2(q)\left(1 + \frac{\rho'}{x^2}\eta(x)\right)^{-2}; \tag{21}$$

$$\eta(x) = -\frac{2\pi^2 T'_F}{p_F^2}\Pi(2p_{Fx};0) = 1 + \frac{1-x^2}{2x}\ln\frac{1+x}{1-x}; \tag{22}$$

$$\rho = p_F^2 g^2/2\pi^2 T'_F, \qquad \rho' = e^2/2\pi T'_F, \qquad x = q/2p_F. \tag{23}$$

These formulas show that the Coulomb interaction enters in screened form and, moreover, leads to a renormalization of the phonon frequencies and of the bare coupling constant g.

Using these approximate formulas, we can perform the integration over p_1^0. Further integration over the variable p_1 leads, at $\omega = 0$, to a logarithmic divergence on the Fermi surface. This circumstance is used to determine the magnitude of ω with asymptotic accuracy as $B(qq^0) \to 0$. Integration by parts makes it possible to isolate the logarithmic singularity. In this way we obtain $(U(p \mid p^0) = U(p_F \mid 0)\varphi(p \mid p^0))$:

$$\varphi_\omega(p \mid p^0) = Z^2(p_F)\frac{mp_F}{4\pi^2}\,\bar{B}(pp_F \mid p^0)(\ln\omega^2 - i\pi) + \sum_{i=1}^{3} A_i(p \mid p^0); \tag{24}$$

where

$$A_1(p \mid p^0) = -\frac{m}{4\pi^2}\int_0^{p_F} \ln T(p_1)\, d\{p_1 Z^2(p_1)\bar{B}(pp_1 \mid p^0 - T(p_1))\varphi_\omega(p_1 \mid T(p_1))\};$$

$$A_2(p \mid p^0) = \frac{m}{4\pi^2} \int_{p_F}^{\infty} \ln T(p_1)\, d\{p_1 Z^2(p_1) \bar{B}(pp_1 \mid p^0 + T(p_1)) \varphi_\omega(p_1 \mid -T(p_1))\};$$

$$A_3(p \mid p^0) = \frac{1}{16\pi^3} \int_0^{\infty} p_1^2\, dp_1\, d\Omega\, g_e^2(p-p_1) \omega_e(p-p_1) G(p^0 - \omega_e(p-p_1) \mid p_1) \times$$

$$\times G(-p^0 + \omega_e(p-p_1) \mid -p_1) \varphi_\omega(p_1 \mid p^0 - \omega(p-p_1));$$

$\bar{B}$ is the average over the angular variables. Denoting

$$\tilde{\rho} = -\frac{mp_F}{2\pi^2} Z^2(p_F) \bar{B}(p_{F_p} F \mid 0), \qquad \tilde{\rho} \ln \tilde{\omega} = \sum_{i=1}^{3} A_i(p_F \mid 0), \tag{25}$$

we obtain

$$\omega = i\tilde{\omega} \exp(-1/\tilde{\rho}). \tag{26}$$

On the basis of (26), the energy of the collective excitation of a pair of particles with opposite momenta has turned out to be imaginary, which, as has already been noted, corresponds to the instability of the normal state of the metal and, consequently, to the realization of the superconducting state. The assumption made that ω is small is justified if $\tilde{\rho}$ is a small positive quantity:

$$\tilde{\rho} > 0. \tag{27}$$

This inequality is thus a criterion of superconductivity.

Along with this, there exists a second inequality, $\omega_e^2(q) \geq 0$ for all values of q bounded by the maximum Debye momentum q_m. It corresponds to the reality of the observable quantity ω_e and, consequently, to the stability of the crystal lattice with respect to one-phonon excitations.

arguments ([9]). On the basis of (20) we have the inequality

$$x^2 + \eta(x)(\rho' - \rho x^2) > 0, \tag{28}$$

which must be satisfied for all x in the interval $(0, x_m)$, where $x_m = q_m/2p_F$. (28) imposes an upper bound on the seed parameters ρ and g:

$$\rho < \rho_0, \qquad \rho_0 = \min(\rho'/x^2 + 1/\eta(x)). \tag{29}$$

For $\rho' = 0$, i.e., in the case when the Coulomb interaction between electrons is not taken into account, criterion (29) takes the form

$$\rho < 0.5, \tag{30}$$

since the largest value of the function $\eta(x)$ is $\eta(0) = 2$; (30) coincides with the criterion of work ([9]).

Let us now return to the criterion of superconductivity. On the basis of (25) and (17)–(20) we have:

$$\tilde{\rho} = \int_0^a 2x(\rho x^2 - \rho')\,[x^2 + \eta(x)(\rho' - \rho x^2)]^{-1}\,dx > 0, \tag{31}$$

where the smaller of the two numbers x_m and 1 is taken as the upper limit of integration. This inequality obviously means a lower bound on the constant ρ. Replacing in formula (31) the monotone function $\eta(x)$ by its smallest value $\eta_m = \eta(a)$ and carrying out the integration, we obtain the sufficient criterion of superconductivity

$$(1 - \rho\eta_m)^{-2}\left[a\rho(1 - \rho\eta_m) - \rho' \ln\left(1 + \frac{1 - \rho\eta_m}{\rho'\eta_m}a^2\right)\right] > 0; \tag{32}$$

taking into account the smoothness of the function $\eta(x)$ in the interval under consideration, one may expect that (32) is close to (31).

The sufficient criterion of superconductivity (32), together with the condition of stability of the crystal lattice (28), means that

$$1/\eta_m - \varepsilon\rho'/a^2 < \rho < \rho_0, \tag{33}$$

where ε is the root of the equation

$$\frac{1}{\varepsilon} - \frac{\rho'\eta_m}{a^2} - \frac{1}{\varepsilon^2}\ln(1 + \varepsilon) = 0, \qquad \varepsilon > -1. \tag{34}$$

The author takes this opportunity to express his deep gratitude to Acad. N. N. Bogolyubov, D. N. Zubarev, S. V. Tyablikov, and Yu. A. Tserkovnikov for useful advice and discussion of the results.

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Received
24 V 1962

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