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Abstract

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PHYSICS

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ON ALLOWING FOR THE COULOMB INTERACTION IN A TWO-BAND MODEL OF A SUPERCONDUCTOR

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Until now, the influence of the Coulomb interaction between electrons on the value of the critical temperature of a superconductor has been considered only in a one-band model. In the present work this interaction is taken into account within the framework of a two-band model of a pure superconductor with a nonmagnetic impurity.

We shall start from the Bardeen-Pines Hamiltonian ⁽¹⁾ for a two-band model. In this case the Bloch functions $\psi_{nk}(x)$ are used as the basis functions of the second-quantization representation. This Hamiltonian, which takes into account the electron-phonon and electron-electron interactions ⁽²⁾, can be represented in the form

$$H = H_0 + H_i, \quad (1)$$

where

$$H_0 = H_e + H_{ph} + H_c, \quad H_i = \sum_{\sigma} \int dx \psi^+(x\sigma) \psi(x\sigma) \Phi(x), \quad (2)$$

$$\Phi(x) = \Phi_{ph}(x) + \Phi_c(x), \quad \Phi_{ph}(x) = \sum_q \frac{A_q}{\sqrt{2\Omega_q}} (b_q + b_{-q}^+) e^{iqx},$$

$$A_q = -\frac{4\pi Ze^2}{q} \sqrt{\frac{n_i}{VM}}.$$

The phonon frequencies Ω_q depend only weakly on the momentum and may be replaced by the ionic plasma frequency Ω_p :

$$\Omega_p = (4\pi Z^2 e^2 n_i / M)^{1/2}. \quad (3)$$

Ze , M , n_i are, respectively, the charge, mass, and density of the ions; H_c and Φ_c are the free Hamiltonian and the amplitude of the auxiliary quantum field, with Φ_c satisfying the condition

$$\langle T\Phi_c(x)\Phi_c(x') \rangle = -v(x-x')\delta(\tau-\tau'), \quad (4)$$

where $v(x)$ is the energy of the Coulomb interaction of the electrons.

For the one-particle electron Green's function of a pure superconductor the simplest approximation is used,

$$G_n(k|\Omega) = (E_n(k) - i\Omega)^{-1}. \quad (5)$$

Let us consider the one-particle boson Green's function

$$B(x, x') = \langle T\Phi(x)\Phi(x')u \rangle / \langle u \rangle. \quad (6)$$

Since, when transfer processes are neglected, the quasimomentum is conserved, the equation for the function B in the two-band case has the same form as in the one-band model:

$$B(q) = B_0(q)/(1 - B_0(q)\Pi(q)), \quad (7)$$

where in the present case $\Pi(q)$ has the form

$$\Pi(\mathbf{q}|\omega) = -\frac{2}{\beta V} \sum_{nm} \sum_{k\Omega} G_n(\mathbf{k}|\Omega) G_m(\mathbf{k}-\mathbf{q}|\Omega-\omega) |\chi(n\mathbf{k}; m\mathbf{k}-\mathbf{q})|^2 = \frac{2}{V} \sum_k \sum_{nm} \bar{n}_n(k) |\chi(n\mathbf{k}; m\mathbf{k}-\mathbf{q})|^2 \left(\frac{1}{E_m(\mathbf{k}-\mathbf{q})} - \frac{1}{E_n(\mathbf{k})} \right)$$

$\chi(n\mathbf{k}; n'\mathbf{k}')$ is the integral over the elementary cell of two modulating factors of the Bloch functions $(u_{n\mathbf{k}}^*(x)u_{n'\mathbf{k}'}(x))$, and $\bar{n}_n(k)$ is the mean number of electrons in the n -th band.

In the region of small q , the most substantial contribution is made by the terms of the sum with $n = m$. In what follows we shall need the function B in the region of small frequencies ω and small q . In this case the quantity $\Pi(q)$ may be replaced by $\Pi(0|0)$. The function $B^0(q)$ is equal to:

$$B^0(q) = v(q)\Omega_p^2/(\Omega_p^2 + \omega_n^2) - v(q), \quad (9)$$

where the relation $VA_q^2 = \Omega_p^2 v(q)$, valid by virtue of definitions (2) and (3), has been used. On the basis of (7) and (9) we have

$$B(q) = D(q) - V_c(q), \quad (10)$$

where

$$D(q) = V_c(q)\omega^2(q)/(\omega^2(q) + \omega_n^2), \quad V_c(q) = v(q)/K(q),$$

$$\omega^2(q) = \Omega_p^2/K(q), \quad K(q) = 1 + v(q)\Pi(q). \quad (11)$$

In the region $q \rightarrow 0$, $\omega = 0$, we have

$$K(q) \simeq 1 + k_s^2/q^2 \simeq k_s^2/q^2, \quad k_s^2 = 4\pi e^2 \Pi(0|0), \quad (12)$$

and, consequently,

$$\omega^2(q) \simeq q^2 s^2, \quad s = |\Omega_p|/k_s, \quad (13)$$

i.e., the usual dispersion law of an acoustic wave with velocity s is obtained.

On the basis of (3), the critical temperature of a pure superconductor in the two-band model is determined from the equation:

$$F(x, y) = \int d^4x_1 d^4x_2 G(x, x_1) G(y, x_2) B(x_1, x_2) F(x_1, x_2), \quad (14)$$

which is transformed into the form

$$u_n(\mathbf{k}|\Omega) = \frac{1}{\beta V} \sum_{n_1} \sum_{\mathbf{k}_1 \Omega_1} B(\mathbf{k}-\mathbf{k}_1|\Omega-\Omega_1) |\chi(n\mathbf{k}; n_1 \mathbf{k}_1)|^2 \times G_{n_1}(\mathbf{k}_1|\Omega_1) G_{n_1}(-\mathbf{k}_1|-\Omega_1) u_{n_1}(\mathbf{k}_1|\Omega_1). \quad (15)$$

Using formula (10) and the possibility of taking certain factors out on the Fermi surface, we obtain:

$$u_n(\Omega) = \frac{\pi}{\beta} \sum_{n_1} \sum_m \frac{1}{|\Omega_1|} [D_{nm}(\Omega - \Omega_1) - V_{nm}^c] N_m u_m(\Omega_1), \quad (16)$$

where N_m is the density of electronic states on the m -th sheet of the Fermi surface. The definition of D_{nm} and V_{nm}^c coincides with the definition of the quantities V_{nm} in work (3).

The quantities V_{nm}^c are regarded as independent of Ω in a bounded frequency interval $(-E_m^c, E_m^c)$, where E_m^c is of the order of the Fermi energy. After separating out the logarithmic singularities, we obtain

$$\tilde{u}_n(x) = \sum_m \ln \frac{2\gamma\beta\Omega_{nm}}{\pi} [\tilde{D}_{nm}(x) - V_{nm}^c] N_m \tilde{u}_m(0) - \sum_m V_{nm}^c N_m \ln \left(\frac{E_m^c}{\Omega'_{nm}} \right) \tilde{u}_m(E_m^c). \quad (17)$$

The quantities Ω_{nm} and Ω'_{nm} are subsequently replaced by the Debye frequency, and therefore are not given here. Such a replacement apparently does not substantially affect the determination of the critical temperature T_c and the magnitude of the isotope effect. Functions with a wavy bar are equal to the half-sum of functions with arguments $x + i\delta$ and $x - i\delta$.

Setting $x = 0$ and $x = E_n^c$ ($n = 1, 2$) in equation (17), we obtain a system of 4 equations from which the quantity T_c is determined. From the compatibility condition of this system we obtain the equation ($C \neq 0$)

$$a_0 \xi^2 - b_0 \xi + 1 = 0, \quad (18)$$

for determining the positive quantity ξ

$$\xi = \ln \frac{2\gamma\beta_c \omega_D}{\pi} = \frac{b_0 \pm \sqrt{b_0^2 - 4a_0}}{2a_0}, \quad (19)$$

and thereby the critical temperature of the superconductor

$$T_{c0} = \frac{2\gamma}{\pi} T_D e^{-\xi_{\pm}}, \quad (20)$$

where

$$b_0 = N_1 \Gamma_{11} + N_2 \Gamma_{22}, \quad a_0 = N_1 N_2 (\Gamma_{11} \Gamma_{22} - \Gamma_{12} \Gamma_{21}),$$

$$\Gamma_{11} = D_{11} - \frac{V_{11}^c}{(1 + V_{11}^c N_1 \eta_1)} + \frac{V_{12}^c V_{21}^c N_2 \eta_2}{(1 + V_{11}^c N_1 \eta_1) C}, \quad (21)$$

$$\Gamma_{12} = D_{12} - \frac{V_{12}^c}{C}, \quad \eta_n = \ln \frac{E_n^c}{\hbar \omega_D},$$

$$C = (1 + V_{11}^c N_1 \eta_1)(1 + V_{12}^c N_2 \eta_2) - N_1 N_2 V_{12}^c V_{21}^c \eta_1 \eta_2. \quad (22)$$

The quantities Γ_{22} and Γ_{21} are determined analogously. On the basis of the last formulas we obtain the following formula for the isotopic change of the critical temperature:

$$\frac{\delta T_c}{T_c} = -\frac{1}{2} \frac{\delta M}{M} (1 - \zeta),$$

where

$$\zeta_{\pm} = \pm \frac{1}{a_0 \sqrt{b_0^2 - 4a_0}} \{[\xi_{\pm}(2a_0\xi_{\pm} - b_0) + 1]\gamma_1 - a_0\xi_{\pm}\gamma_2\},$$

$$\gamma_1 = -N_1 N_2 \{\Gamma_{11} N_2 (\Gamma_{22} - D_{22})^2 + \Gamma_{22} N_1 (\Gamma_{11} - D_{11})^2 + \frac{(D_{12} V_{21}^c + D_{21} V_{12}^c)}{C} [N_1 (\Gamma_{11} - D_{11}) + N_2 (\Gamma_{22} - D_{22})] - \dots\}$$

$$\gamma_2 = - \left[N_1^2 (\Gamma_{11} - D_{11})^2 + N_2^2 (\Gamma_{22} - D_{22})^2 + \frac{2V_{12}^c V_{21}^c N_1 N_2}{C^2} \right].$$

If the quantities determining interband transitions are small,⁴ and may be neglected, then the two bands are independent, and in each of them its own critical temperature is established. Thus, for example, in the first band we have

$$\xi_1 = (N_1 \Gamma_{11})^{-1}, \quad \zeta_1 = \left(\frac{\Gamma_{11} - D_{11}}{\Gamma_{11}} \right)^2, \quad \Gamma_{11} = D_{11} - V_{11}^c / (1 + V_{11}^c N_1 \eta_1). \quad (24)$$

These formulas coincide with the results of works^{5,6}, in which the influence of Coulomb interaction on the critical temperature of pure superconductors in the one-band model is taken into account.

We note that in works⁽²⁾ the question of the role of the Coulomb interaction was also considered on the basis of the Fröhlich model supplemented by the Coulomb interaction. Since the Fröhlich model already partially takes the Coulomb interaction into account, such a treatment is not correct. The correct allowance for the Coulomb interaction of electrons is possible on the basis of the Bardeen-Pines Hamiltonian, and, thus, the results of the present work, corresponding to the one-band approximation, should be regarded as a correction to the final results of the works⁽²⁾.

Let us dwell briefly on the question of the criterion for superconductivity in a two-band metal model. In those cases where equation (18) has no positive solutions, the metal is nonsuperconducting. From formula (19) it is seen that $\xi_{\pm} < 0$ if the parameters of the substance a_0 and b_0 satisfy the conditions $a_0 \geq 0$, $b_0 \leq 0$.

In the general case, when the parameters D_{ij} and V_{ij}^c are not equal to one another, the question of the compatibility of these two conditions remains open. However, for the Bardeen-Pines Hamiltonian used by us, by virtue of formulas

(10) and (11), the equalities $D_{ij} = V_{ij}^c$ hold (which are apparently special cases of a more general situation). In this case it is more convenient to proceed not from expressions (18) and (19), but from the formulas

$$a\xi^2 - b\xi + C \neq 0, \quad \xi_{\pm} = (b \pm \sqrt{b^2 - 4ac})/2a,$$

$$a = Ca_0, \quad b = Cb_0, \quad a = N_1^2 N_2^2 \eta_1 \eta_2 (V_{11}^c V_{22}^c - V_{12}^c V_{21}^c)^2 \geq 0. \quad (25)$$

It then turns out that there always exists a positive solution for ξ , and consequently in the two-band Bardeen-Pines model superconductivity always exists.

Let us consider briefly the question of the influence of the Coulomb interaction between electrons on the formulas of the impurity theory of superconductivity set forth in ⁽³⁾. A detailed investigation of this question shows that all final formulas of work ⁽³⁾ remain valid also in the present case, provided only that the quantities D_{ij} of work ⁽³⁾ (there they are denoted by V_{ij}) are replaced by the quantities Γ_{ij} according to formulas (21).

Thus, for the critical temperature of a superconductor with impurity we obtain the expressions

$$\ln \frac{\beta_c}{\beta_{c0}} = \alpha^{\pm} \left\{ \psi \left[\frac{1}{2} + \frac{\hbar\beta_c}{4\pi} \left(\frac{1}{\tau_{12}} + \frac{1}{\tau_{21}} \right) \right] - \psi(1/2) \right\},$$

$$\alpha^{\pm} = \frac{1}{2} \left\{ 1 \pm \frac{\frac{N_2 - N_1}{N_1 + N_2} (\Gamma_{22} N_2 - \Gamma_{11} N_1) + \frac{2N_1 N_2}{N_1 + N_2} (\Gamma_{12} + \Gamma_{21})}{\sqrt{b^2 - 4a}} \right\}; \quad (26)$$

$\beta_{c0} = (kT_{c0})^{-1}$ is determined by formula (20). The coefficient $\alpha^{\pm}$ takes a value between zero and unity.

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