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DETERMINATION OF THE CRITICAL TEMPERATURE OF A SUPERCONDUCTOR WITH AN ELECTRIC IMPURITY

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In the work of A. A. Abrikosov and L. P. Gor' kov [1], it was shown, using the example of the one-band model of Bardeen, Cooper, and Schrieffer [2], that an electric impurity does not exert a noticeable influence on the critical temperature T_c of a superconductor, and that such an influence is exerted by a paramagnetic impurity.

In the present work a two-band model of a superconductor is considered on the basis of the Fröhlich Hamiltonian, and it is assumed that the impurity is electric. We shall show that, owing to interband scattering by the impurity, a substantial change in T_c occurs.

For the proof we shall use the method for determining the temperature T_c proposed in [3], which we shall supplement, on the one hand, by taking into account band overlap, according to [4] (see also [5]), and, on the other hand, by taking the impurity into account. We note that in what follows we neglect transfer processes and use the weak-coupling approximation.

According to [3], the critical temperature of a superconductor is regarded as the temperature at which the superconducting phase nucleates. It is found as the eigenvalue of the equation for the bound state of a pair of electrons or holes when their binding energy is equal to zero.

In the presence of an impurity this equation has the form

$$F(x\alpha, y\beta) =$$

$$= \int \dots \int K(xy;12) \sum_{\sigma\sigma'} \sigma(1\alpha 2\beta; 3\sigma 4\sigma')\, F(3\sigma, 4\sigma')\, d^4 1 \dots d^4 4; \qquad (1)$$

$x = (\mathbf{x}, \tau)$, α is a spin variable.

The function K, first introduced in [1], is defined as the average, over the positions of the randomly distributed impurity, of the product of two electron temperature Green’ s functions.

$$K(xy;12) = \overline{G}(x1)\,\overline{G}(y2); \tag{2}$$

σ is the compact mass operator of this equation, containing, along with phonon lines, also impurity lines. The function K satisfies the equation

$$K(xy;12) = \overline{G}(x1)\overline{G}(y2) + \int \dots \int \overline{G}(x3)\overline{G}(y4)I(34;56)K(56;12)d^4 3 \dots d^4 6. \tag{3}$$

In what follows we use the simplest approximations for the functions σ and I:

$$\sigma(1\alpha 2\beta; 3\sigma 4\sigma') = B^0(1-2)\delta^4(1-3)\delta^4(2-4)\delta_{\alpha\sigma}\delta_{\beta\sigma'},$$

$$I(34;56) = \frac{c}{V}\sum_q |u(q)|^2 e^{-iq(3-4)}\delta^4(3-5)\delta^4(4-6), \tag{4}$$

where B^0 is the zero phonon (temperature) Green’ s function; $u(\mathbf{q})$ is the Fourier image of the impurity-interaction potential.

In the band case, it is evidently convenient to use expansions in Bloch functions

$$\psi_{n\mathbf{k}}(\mathbf{r}) = \sqrt{V_0/V}\, e^{-i\mathbf{kr}} u_{n\mathbf{k}}(\mathbf{r}),$$

where V is the volume of the system, V_0 the volume of the elementary cell.

In the case of overlapping energy bands (in our case, two bands), the Fermi surface consists of two sheets corresponding to the different bands. We shall assume approximately that the sheets are spherical and have Fermi radii k_1^F and k_2^F (determined from the conditions $E_1(k_1^F) = E_2(k_2^F) = 0$). We shall assume that the first band is broad (the conduction band) and the second narrow (for example, a d-band). Denoting by μ the chemical potential of the system, we may write $E_1(k_2^F) \approx \mu$; $E_2(k_1^F) \approx \frac{m_1}{m_2}\mu$, where m_i are the effective masses of the electrons ($m_1 < m_2$). Under these assumptions, a sufficiently good approximation for the ($n\mathbf{k}$)-representation of the Green’ s function $\widetilde{G}$, averaged over the impurity positions, is the formula

$$\widetilde{G}(n\mathbf{k}, n'\mathbf{k}'|\Omega) = \delta_{k,\mathbf{k}'}\delta_{n,n'}\widetilde{G}_n(\mathbf{k}|\Omega), \qquad \widetilde{G}_n(\mathbf{k}|\Omega) = \left(E_n(\mathbf{k}) - i\Omega\eta_n\right)^{-1}, \tag{5}$$

where

$$\eta_n(\Omega) = 1 + \frac{\hbar}{2\tau_n|\Omega|}; \qquad \frac{1}{\tau_n} = \frac{1}{\tau_{n1}} + \frac{1}{\tau_{n2}}, \tag{6}$$

$$\frac{\hbar}{2\tau_{ij}} = \frac{c\pi}{(2\pi\hbar)^3} \int_{S_m} \frac{dS_m}{|\nabla E_m|} \left|u(\mathbf{k}_n^F - \mathbf{k}_m^F)\right|^2 \left|\chi(n\mathbf{k}_n, m\mathbf{k}_m)\right|^2,$$

$$\chi(n\mathbf{k}, m\mathbf{k}') = \int_{V_0} u^*_{n\mathbf{k}} u_{m\mathbf{k}'} \, d\mathbf{r};$$

S_m is the surface of the m-th sheet; c is the impurity concentration. For the $(n\mathbf{k})$-representations of the functions F and K, and (taking account of the conservation laws of quasimomenta), on the basis of (1) and (3) we obtain

$$F_{nn'}(\mathbf{k}|\Omega) = \frac{1}{\beta^2 V} \sum_{\Omega'\Omega''} \sum_{n_1 \ldots n_4} \sum_{k_1 \mathbf{k}_2} B(\mathbf{k}_1 - \mathbf{k}_2|\Omega' - \Omega'') K_{nn'n_1n_2}(\mathbf{k}\mathbf{k}_1|\Omega, \Omega') \times$$

$$\times \chi(n_1\mathbf{k}_1, n_3\mathbf{k}_2)\chi^*(n_2\mathbf{k}_1, n_4\mathbf{k}_2) F_{n_3n_4}(\mathbf{k}_2|\Omega''); \tag{7}$$

$$K_{n_1n_2n_3n_4}(\mathbf{k}\mathbf{k}'|\Omega\Omega') = \widetilde{G}_{n_1}(\mathbf{k}|\Omega)\widetilde{G}_{n_2}(-\mathbf{k}|-\Omega)[\beta\delta_{\Omega,\Omega'}\delta_{k,\mathbf{k}'}\delta_{n_1n_3}\delta_{n_2n_4} +$$

$$+ \frac{c}{V}\sum_{k_1} \left|u(\mathbf{k} - \mathbf{k}_1)\right|^2 \sum_{m_1m_2} \chi(n_1\mathbf{k}, m_1\mathbf{k}_1)\chi^*(n_2\mathbf{k}, m_2\mathbf{k}_1) K_{m_1m_2;n_3n_4}(\mathbf{k}_1\mathbf{k}'|\Omega\Omega')]. \tag{8}$$

From the last equation it follows that the functions K may be sought in the form of the product $\delta_{\beta\Omega,\Omega'}\widetilde{G}_{n_1}(k|\Omega)\widetilde{G}_{n_2}(-k|-\Omega)$ by some new function L. Obviously, the functions $F_{nn'}$ should also be sought in the form of the product of Green' s functions by some new function $f_{nn'}$. The system of equations for the new functions introduced in this way can be substantially simplified if one takes into account that the products of the Green' s functions $\widetilde{G}_{n_1}\widetilde{G}_{n_2}$ are most significant for $n_1 = n_2$. With this approach to these equations it is found that, although the functions $f_{nn'}$ nondiagonal in the band numbers are not equal to zero, nevertheless the critical temperature T_c is determined only by the diagonal elements f_{nn}. Taking further into account that, alongside the product of Green' s functions, the remaining factors may be taken out onto the Fermi surfaces,

under the assumption of isotropic solutions we obtain the system of equations

$$f_r(\Omega) = \frac{\pi}{\beta} \sum_{\Omega'} \sum_{m} L_{rm}(\Omega\Omega')\, N_m \Lambda_m(\Omega')\, f_m(\Omega'); \tag{9}$$

$$L_{rm}(\Omega, \Omega') = 4\pi V_{rm}(\Omega - \Omega') + \sum_{n} \frac{\hbar}{2\tau_{rn}} \Lambda_n(\Omega) L_{nm}(\Omega, \Omega'), \tag{10}$$

where

$$V_{rm}(\Omega - \Omega') N_m = \frac{1}{(2\pi)^3} \int_{S_m} \frac{dS_m}{|\nabla E_m|} B(\mathbf{k}_r^F - \mathbf{p}_m^F \mid \Omega - \Omega')\, |\chi(r\mathbf{k}_r^F, m\mathbf{p}_m^F)|^2, \tag{11}$$

$$N_m = \frac{1}{2\pi^2} \left(\frac{k^2}{|\nabla E_m|} \right)_{k=k_m^F}$$

is the density of states on the m-th sheet of the Fermi surface; further,

$$\Lambda_n(\Omega) = \frac{1}{\pi} \int dE_n\, \widetilde{G}_n(k \mid \Omega) \widetilde{G}_n(-k \mid -\Omega) = \frac{1}{\pi \eta_n(\Omega)}. \tag{12}$$

Solving the system (10) presents no difficulty. Substituting the functions L_{rn} found from (9) and introducing new functions X_i by the formula

$$X_i(\Omega) = \frac{\pi}{\beta} \sum_{\Omega'} [V_{i1}(\Omega - \Omega') N_1 \Lambda_1(\Omega') f_1(\Omega') + V_{i2}(\Omega - \Omega') N_2 \Lambda_2(\Omega') f_2(\Omega')], \tag{13}$$

we obtain the system of equations ($i = 1, 2$)

$$\begin{aligned} X_i(\Omega) = & \frac{\pi}{\beta} \sum_{\Omega'} \frac{1}{|\Omega'|} [V_{i1}(\Omega - \Omega') N_1 X_1(\Omega') + V_{i2}(\Omega - \Omega') N_2 X_2(\Omega')] + \\ & + \frac{\pi}{\beta} \sum_{|\Omega'|} \frac{N_1}{|\Omega'|} \frac{(X_1(\Omega') - X_2(\Omega'))(V_{i2}(\Omega - \Omega') j - V_{i1}(\Omega - \Omega'))}{1 + \tau_{12}/\tau_{21} + 2\tau_{12}|\Omega'|/\hbar}, \end{aligned} \tag{14}$$

$$j = \frac{N_2}{N_1} \frac{\tau_{12}}{\tau_{21}}.$$

The system of equations (14) is solved in the limiting case of weak coupling (small V_{ij} and large β_c). Using the method of extracting the leading logarithmic terms in β_c, developed in the works of N. N. Bogolyubov ([6]) and D. N. Zubarev and Yu. A. Tserkovnikov ([7]), we obtain ($X_i \equiv X_i(\delta)$; $V_{ij} \equiv V_{ij}(\delta)$, $\delta \to 0$):

$$X_i = \ln\left(\frac{2\gamma\beta_c}{\pi}\right)(V_{i1}N_1X_1 + V_{i2}N_2X_2) + V_{i1}N_1X_1 \ln\hbar\omega_{i1} +$$

$$+V_{i2}N_2X_2 \ln\hbar\omega_{i2} + \frac{N_1(X_1 - X_2)}{1 + \tau_{12}/\tau_{21}}(V_{i2}j - V_{i1})I, \tag{15}$$

where

$$I = \int_0^\infty \frac{dt}{t}\,\frac{\text{th}\left[\frac{1}{4}\hbar\beta_c\left(\frac{1}{\tau_{12}} + \frac{1}{\tau_{21}}\right)t\right]}{1 + t^2} = \psi\left(\frac{1}{2} + \frac{\hbar\beta_c}{4\pi}\left(\frac{1}{\tau_{12}} + \frac{1}{\tau_{21}}\right)\right) - \psi(1/2); \tag{16}$$

$$\ln\hbar\omega_{ij} = -\int_0^\infty \ln y\, d\frac{[(V_{ij}(\delta - iy) + V_{ij}(-\delta - iy))N_j(X_j(iy + \delta) + X_j(iy - \delta))]}{4V_{ij}N_{jX}j}. \tag{17}$$

On the basis of (15) one can show that

$$\ln\frac{\beta_c}{\beta_{c0}} = A + B, \tag{18}$$

where

$$A = \frac{N_1 I}{D(1 + \tau_{12}/\tau_{21})}\left[(V_{22}j - V_{21})(1 - V_{11}N_1\xi_{11} - V_{12}N_2\xi_{12}) +\right.$$

$$\left.+(V_{12}j - V_{11})(V_{21}N_1\xi_{21} + V_{22}N_2\xi_{22} - 1)\right]; \tag{19}$$

$$D = V_{11}N_1(1 - V_{22}N_2\xi_{22}) + V_{22}N_2(1 - V_{11}N_1\xi_{11}) + V_{12}V_{21}N_1N_2(\xi_{12} + \xi_{21}); \tag{20}$$

$$\xi_{ij} = \ln\left(\frac{2\gamma\beta_{c0}\hbar\omega^0_{ij}}{\pi}\right). \tag{21}$$

Quantities for the pure superconductor are denoted by the subscript zero. The quantity B, proportional to $\ln\omega_{ij}/\omega^0_{ij}$, is apparently less significant than A, and therefore is not written out here. Retaining in A only the terms that do not vanish as $V_{ij} \to 0$, we obtain

$$A = \alpha^{\pm} I,$$

$$\alpha^{\pm} = \mp \frac{N_1 \left[V_{11} + V_{22} j - V_{21} - V_{12} j - \frac{N_1 j + N_2}{2 N_1 N_2} \left(b_0 \pm \sqrt{b_0^2 - 4a} \right) \right]}{(1 + \tau_{12}/\tau_{21}) \sqrt{b_0^2 - 4a}}, \quad (22)$$

where

$$b_0 = V_{11} N_1 + V_{22} N_2, \qquad a = N_1 N_2 (V_{11} V_{22} - V_{12} V_{21}). \quad (23)$$

For $j = 1$, $\alpha^{\pm}$ may take a value between zero and unity. On the basis of (18) and (22), in the region of low impurity concentrations we obtain a linear decrease of the critical temperature with increasing impurity,

$$T_c \simeq T_{c0} - \frac{1}{8} \pi \hbar \alpha^{\pm} (1/\tau_{12} + 1/\tau_{21}). \quad (24)$$

In the region of high impurity concentrations, $\beta_c \tau_{12}^{-1} \gg 1$, β_c increases with increasing impurity concentration; moreover, the critical impurity concentration at which $T_c = 0$ is observed only under the condition $\alpha^{\pm} = 1$.

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