TWO-BAND-MODEL DETERMINATION OF THE CRITICAL TEMPERATURE OF A SUPERCONDUCTOR WITH AN IMPURITY

V. A. MOSKALENKO and M. E. PALISTRANT

Moscow State University; Mathematics Institute, Academy of Sciences, Moldavian S.S.R.

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The effect of a nonmagnetic impurity on the critical temperature T_c of a superconductor with overlapping energy bands is investigated. It is shown that a significant change in the magnitude of T_c is produced by interband scattering of electrons by the impurity. The extreme cases of small and large impurity concentrations are investigated. In the former, an increase of concentration is accompanied by a linear decrease of T_c. The proof is based on the definition of the critical temperature as the eigenvalue of the equation for bound pair production. The calculations are performed in the weak electron-phonon coupling approximation and by neglecting single-particle Green's-function elements that are nondiagonal with respect to the band indices.

1. INTRODUCTION

THE influence of impurities on the critical temperature T_c of superconductors has heretofore been investigated on the basis of the single-band model of Bardeen, Cooper, and Schrieffer [1]. Abrikosov and Gor'kov [2] have shown with this model that a paramagnetic impurity exerts an appreciable influence on the critical temperature, whereas a nonmagnetic impurity has no such effect. Markowitz and Kadanoff [3] started from Bardeen's anisotropic single-band model and investigated the influence of a nonmagnetic impurity on T_c. They have shown that the scattering of the electrons by the impurity smoothes out the anisotropy of the energy gap and lowers the critical temperature. By choosing the anisotropy parameter it is possible to reconcile their theory with the experimental data [4].

In many superconducting metals, overlap of two or more energy bands is observed near the Fermi energy. In this case, the single-band approximation is insufficient. We consider in this article the influence of a nonmagnetic impurity on T_c in a two-band model and show that this influence is appreciable, owing to the interband scattering of the electrons by the impurity. We use for the proof the previously developed method [5] of determining the critical temperature of a superconductor, and a generalization of the results of the theory of pure superconductors with overlapping energy bands, contained in our earlier paper [6] and in that of Suhl, Matthias, and Walker [7]. The influence of a nonmagnetic impurity on T_c is investigated under the assumption of weak electron-photon coupling and without account of Umklapp processes.

2. ELECTRONIC GREEN'S FUNCTION OF A NORMAL METAL WITH NONMAGNETIC IMPURITY

The operator of the interaction between electrons and an impurities randomly situated at the points $\mathbf{r}_j$ is of the form

$$H_{\text{imp}}=\frac{1}{V}\sum_{\substack{\mathbf{k}\mathbf{k}'\sigma\\ nn'}} u(\mathbf{k}-\mathbf{k}')\,\rho(\mathbf{k}-\mathbf{k}')\,\chi(n\mathbf{k}\,n'\mathbf{k}')\,a^{+}_{n\mathbf{k}\sigma}a_{n'\mathbf{k}'\sigma}, \quad (1)$$

where

$$\chi(n\mathbf{k}\,n'\mathbf{k}')=\int_{V_0} u^{*}_{n\mathbf{k}}(r)\,u_{n'\mathbf{k}'}(\mathbf{r})\,d\mathbf{r}, \qquad \rho(\mathbf{r})=\sum_j e^{i\mathbf{k}\mathbf{r}_j}; \quad (2)$$

$u(\mathbf{k})$ is the Fourier transform of the impurity potential, $u_{n\mathbf{k}}(\mathbf{r})$ the modulating factors of the Bloch functions, V the volume of the system, and V_0 the unit-cell volume. The summation over the band indices is confined here and below to two values, in accordance with the choice of the two-band model.

We introduce the electronic temperature Green's function [8]

$$G(n\mathbf{k}\,n'\mathbf{k}'|\tau-\tau')=\langle T a_{n\mathbf{k}}(\tau)a^{+}_{n'k'}(\tau')U(\beta)\rangle/\langle U(\beta)\rangle,$$

$$U(\beta)=T\exp\left(-\int_0^{\beta} H_{\text{imp}}(\tau)\,d\tau\right). \quad (3)$$

In the simplest approximation for the mass oper-

ator $M(nkn'k'|\Omega)$ of this function, after averaging over the impurity positions, we have

$$M(nk\,n'k'|\Omega)=\delta_{kk'}\frac{c}{V}\sum|u(\mathbf{k}-\mathbf{k}_1)|^2G_{n_1}^0(\mathbf{k}_1|\Omega)\times\chi(nk\,n_1\mathbf{k}_1)\chi^{*}(n'\mathbf{k}'\,n_1\mathbf{k}_1),\qquad(4)$$

where c is the impurity concentration;

$$G_n^0(\mathbf{k}|\Omega)=\frac{1}{E_n(\mathbf{k})-i\Omega}$$

$$E_n(\mathbf{k})=T_n(\mathbf{k})-\mu,\qquad\Omega=\frac{(2m+1)\pi}{\beta}$$

$T_n(\mathbf{k})$ is the energy of the particle in the n-th band, and μ is the chemical potential of the system. The averaged Green's function then takes the form

$$\bar{G}(nk\,n'k'|\Omega)=\delta_{kk'}\bar{G}_{nn'}(\mathbf{k}|\Omega);$$

$$\bar{G}_{11}(\mathbf{k}|\Omega)=[E_2(\mathbf{k})-M_{22}(\mathbf{k}|\Omega)-i\Omega][A(\mathbf{k}|\Omega)]^{-1},$$

$$\bar{G}_{22}(\mathbf{k}|\Omega)=[E_1(\mathbf{k})-M_{11}(\mathbf{k}|\Omega)-i\Omega][A(\mathbf{k}|\Omega)]^{-1},$$

$$G_{12}(\mathbf{k}|\Omega)=M_{12}(\mathbf{k}|\Omega)[A(\mathbf{k}|\Omega)]^{-1};$$

$$A(\mathbf{k}|\Omega)=(E_1(\mathbf{k})-i\Omega-M_{11}(\mathbf{k}|\Omega))(E_2(\mathbf{k})-i\Omega-M_{22}(\mathbf{k}|\Omega))-M_{12}(\mathbf{k}|\Omega)M_{21}(\mathbf{k}|\Omega).\qquad(5)$$

In the case of overlapping energy bands, the Fermi surface consists of cavities corresponding to different bands. We assume approximately that in our case the two cavities are nearly spherical in shape and are characterized by two different Fermi radii $\mathbf{k}_1^F$ and $\mathbf{k}_2^F$, determined from the conditions

$$E_1(k_1^F)=0,\qquad E_2(k_2^F)=0.\qquad(6)$$

We assume here that

$$E_2(k_1^F)\sim\mu m_1/m_2,\qquad E_1(k_2^F)\sim\mu,\qquad(7)$$

where m_1, m_2 are the effective masses of the first and second bands near the Fermi level. We take the first band broader than the second and $m_2>m_1$.

It is easy to see that under assumption (7) the function $\tilde{G}_{11}$ is most significant near the first cavity of the Fermi surface, and $\tilde{G}_{22}$ - near the second. The nondiagonal elements $\tilde{G}_{nm}$ are insignificant in this case. In these vicinities, the diagonal elements of the Green's function can be represented as

$$G_{nn}(\mathbf{k}|\Omega)\approx(E_n(\mathbf{k})-i\Omega\eta_n)^{-1};\qquad(8)$$

$$\eta_n=1+\hbar/2\tau_n|\Omega|,\qquad 1/\tau_n=1/\tau_{n1}+1/\tau_{n2};\qquad(8')$$

$$\frac{\hbar}{2\tau_{nm}}=\frac{c\pi}{(2\pi\hbar)^3}\int_{S_m}\frac{dS_m}{|\nabla E_m|}|u(\mathbf{k}_n^F-\mathbf{k}_m^F)|^2|\chi(nk_n^Fmk_m^F)|^2,$$

where S_m is the surface of the m-th cavity. The quantities τ_{nm} are the relaxation times for scattering by the impurity. When n = m the electron remains on the initial cavity of the Fermi surface upon scattering, and when $n\neq m$ the electron jumps over from one cavity to the other. It is precisely these latter processes which produce the change in the critical temperature of the superconductor.

To conclude this section we note that approximation (8) for the Green's function is based on the assumption that the inequality

$$M_{12}/\mu\ll m_1/m_2<1\qquad(9)$$

is satisfied. The relaxation times τ_{nm} (8′) depend, generally speaking, on the orientation of the vector $\mathbf{k}_n^F$. We shall assume henceforth, along with condition (9), that the relaxation times do not depend on the orientations of the vectors $\mathbf{k}_n^F$.

3. FUNDAMENTAL EQUATIONS

The critical temperature of a superconductor is defined as the temperature at which the superconducting phase is created and is the eigenvalue of the equation for the bound state of a pair of electrons or holes with zero binding energy.[5]

To obtain this equation we start from Dyson's equation for the two-particle Green's function of a system described by a Fröhlich Hamiltonian supplemented by the impurity interaction (1) (the Coulomb interaction is not taken into account explicitly):

$$G(x\alpha\,y\beta;\,u\delta\,z\gamma)=G_{\alpha\beta}(xu)G_{\beta\gamma}(yz)-G_{\alpha\gamma}(xz)G_{\beta\delta}(yu)+\sum_{\sigma_1\ldots\sigma_4}\int\ldots\int G_{\alpha\sigma_1}(xx_1)G_{\beta\sigma_2}(yx_2)\Sigma(x_1\sigma_1\,x_2\sigma_2;\,x_3\sigma_3\,x_4\sigma_4)\times G(x_3\sigma_3\,x_4\sigma_4;\,u\delta\,z\gamma)\,d^4x_1\ldots d^4x_4.\qquad(10)$$

All the electron lines of the reduced quantities contain impurity proper-energy inclusions.

We average in this equation over the impurity positions by introducing a new function [2]:

$$K(xy;\,uz)=\overline{G(xu)G(yz)}.\qquad(11)$$

Then the averaged equation (10) takes the form

$$\bar{G}(x\alpha\,y\beta;\,u\delta\,z\gamma)=K(xy;\,uz)\delta_{\alpha\sigma}\delta_{\beta\gamma}-K(xy;\,zu)\delta_{\alpha\gamma}\delta_{\beta\delta}+\sum_{\sigma\sigma'}\int\ldots\int K(xy;\,x_1x_2)\Xi(x_1\alpha x_2\beta;\,x_3\sigma\,x_4\sigma')\times\bar{G}(x_3\sigma\,x_4\sigma';\,u\delta\,z\gamma)\,d^4x_1\ldots d^4x_4,\qquad(12)$$

where the new compact mass operator Ξ, unlike the operator Σ, contains impurity lines besides

the phonon lines. All the electron lines in this equation are in correspondence with function (8).

Since the aforementioned bound state cannot be contained in the inhomogeneous term of (12), it must be left out and then the equation of interest to us takes the form

$$F(x\alpha, y\beta) = \sum_{\sigma\sigma'} \int \dots \int K(xy; x_1x_2)\,\Xi(x_1\alpha\, x_2\beta; x_3\sigma\, x_4\sigma') \times F(x_3\sigma, x_4\sigma')\, d^4x_1 \dots d^4x_4. \quad (13)$$

Abrikosov and Gor'kov [2] obtained for the function K the equation

$$K(xy; x_1x_2) = \bar{G}(xx_1)\bar{G}(yx_2) + \int \dots \int \bar{G}(xx_3)\bar{G}(yx_4) \times I(x_3x_4; x_5x_6) K(x_5x_6; x_1x_2)\, d^4x_3 \dots d^4x_6. \quad (14)$$

The simplest approximations for the functions Ξ and I, which we shall use from now on, are:

$$\Xi(x_1\alpha\, x_2\beta; x_3\sigma\, x_4\sigma') = B(x_1 - x_2)\,\delta^4(x_1 - x_3)\,\delta^4(x_2 - x_4)\,\delta_{\alpha\sigma}\delta_{\beta\sigma'}; \quad (15)$$

$$I(x_3x_4; x_5x_6) = \frac{c}{V}\sum_{\mathbf{q}} |u(q)|^2 e^{-iq(x_3 - x_4)}\delta^4(x_3 - x_5)\,\delta^4(x_4 - x_6), \quad (16)$$

where B(x) is the Green's function of the free phonons.

In our approximation we have ($\alpha = -\beta$)

$$F(xy) = \int d^4x_1\, d^4x_2 K(xy; x_1x_2) B(x_1 - x_2) F(x_1x_2),$$

$$K(xy; x_1x_2) = \bar{G}(xx_1)\bar{G}(yx_2) + \int\int \bar{G}(xx_3)\bar{G}(yx_4) \times \frac{c}{V}\sum_{q} |u(q)|^2 e^{-iq(x_3 - x_4)} K(x_3x_4; x_1x_2)\, d^4x_3\, d^4x_4. \quad (17)$$

Let us expand F and K in terms of the Bloch functions $\psi_{\mathbf{nk}}$. The $\mathbf{nk}$-representations for these functions are denoted by

$$F(n_1\mathbf{k}_1, n_2\mathbf{k}_2|\tau) = \delta_{k_1, -k_2} F_{n_1n_2}(k_1|\tau),$$

$$K(n_1k_1n_2k_2n_3k_3n_4k_4|\tau_x - \tau_1, \tau_y - \tau_2, \tau_1 - \tau_2).$$

The last function is proportional to $\delta_{\mathbf{k}_1 + \mathbf{k}_2, \mathbf{k}_3 + \mathbf{k}_4}$. On the basis of this we obtain

$$F_{nn'}(\mathbf{k}|\Omega) = \frac{1}{\beta^2 V}\sum_{\Omega'\Omega''}\sum_{\substack{n_1 \dots n_4 \\ \mathbf{k}_1\mathbf{k}_2}} B(\mathbf{k}_1 - \mathbf{k}_2|\Omega' - \Omega'') \times K_{nn'n_1n_2}(\mathbf{k}\mathbf{k}_1|\Omega\Omega')\chi(n_1\mathbf{k}_1 n_3\mathbf{k}_2)\chi^*(n_2\mathbf{k}_1 n_4\mathbf{k}_2) \times F_{n_3n_4}(\mathbf{k}_2|\Omega''), \quad (18)$$

where we use the notation

$$K_{nn'n_1n_2}(\mathbf{k}\mathbf{k}_1|\Omega\Omega') = K(n\mathbf{k}\, n' - \mathbf{k}\, n_1\mathbf{k}_1\, n_2 - \mathbf{k}_1|\Omega_1 - \Omega, \Omega - \Omega').$$

In writing out (18) we assume the property $u_{\mathbf{nk}}^*(\mathbf{r}) = u_{\mathbf{n}\,-\mathbf{k}}(\mathbf{r})$.

From (14) we obtain

$$K_{n_1n_2n_3n_4}(\mathbf{k}\mathbf{k}'|\Omega\Omega') = \beta\delta_{\Omega\Omega'}\delta_{\mathbf{k}\mathbf{k}'}\bar{G}_{n_1n_3}(\mathbf{k}|\Omega)\bar{G}_{n_2n_4}(-\mathbf{k}|-\Omega) + \frac{c}{V}\sum_{k_1}|u(\mathbf{k} - \mathbf{k}_1)|^2 \sum_{\substack{m_1m_2 \\ m_3m_4}} \bar{G}_{n_1m_1}(\mathbf{k}|\Omega)\bar{G}_{n_2m_2}(-\mathbf{k}|-\Omega) \times \chi(m_1\mathbf{k}m_3\mathbf{k}_1)\chi(m_2 - \mathbf{k}m_4 - \mathbf{k}_1) K_{m_3m_4n_3n_4}(\mathbf{k}_1\mathbf{k}'|\Omega\Omega'). \quad (19)$$

The system (18) and (19) can be so simplified that the problem of determining the critical temperature of a superconductor in the process of an impurity reduces to a solution of the system of equations (see (A.17) and (A.18) of the Appendix)

$$f_r(\Omega) = \frac{1}{4\beta}\sum_{\Omega'}\sum_{m} L_{rm}(\Omega\Omega')N_m\Lambda_m(\Omega')f_m(\Omega'), \quad (20)$$

$$L_{rm}(\Omega\Omega') = 4\pi V_{rm}(\Omega - \Omega') + \sum_n \frac{\hbar}{2\tau_{rn}}\Lambda_n(\Omega)L_{nm}(\Omega\Omega'). \quad (21)$$

A solution of (21) is obviously

$$L_{rm}(\Omega\Omega') = \Delta_{rm}(\Omega\Omega')/\Delta(\Omega); \quad (22)$$

$$\Delta_{1m}(\Omega\Omega') = 4\pi(V_{1m}(\Omega - \Omega')(1 - \Lambda_2(\Omega)\hbar/2\tau_{22}) + V_{2m}(\Omega - \Omega')\Lambda_2(\Omega)\hbar/2\tau_{12});$$

$$\Delta_{2m}(\Omega\Omega') = 4\pi(V_{2m}(\Omega - \Omega')(1 - \Lambda_1(\Omega)\hbar/2\tau_{11}) + V_{1m}(\Omega - \Omega')\Lambda_1(\Omega)\hbar/2\tau_{21}),$$

$$\Delta(\Omega) = [(1 - \Lambda_1(\Omega)\hbar/2\tau_{11})(1 - \Lambda_2(\Omega)\hbar/2\tau_{22}] - \Lambda_1(\Omega)\Lambda_2(\Omega)\hbar^2/4\tau_{21}\tau_{12}. \quad (23)$$

Substituting this solution in (20) and introducing new functions $\chi_i(\Omega)$ defined by the formulas

$$\chi_i(\Omega) = \frac{\pi}{\beta}\sum_{\Omega'}[V_{i1}(\Omega - \Omega')N_1f_1(\Omega')\Lambda_1(\Omega') + V_{i2}(\Omega - \Omega')N_2f_2(\Omega')\Lambda_2(\Omega')], \quad (24)$$

we obtain

$$\chi_i(\Omega) = \frac{\pi}{\beta}\sum_{\Omega'}\frac{1}{|\Omega'|}[V_{i1}(\Omega - \Omega')N_1\chi_1(\Omega') + V_{i2}(\Omega - \Omega')N_2\chi_2(\Omega')] + \frac{\pi}{\beta}\sum_{\Omega'}\frac{N_1}{|\Omega'|} \times \frac{(\chi_1(\Omega') - \chi_2(\Omega'))(jV_{i2}(\Omega - \Omega') - V_{i1}(\Omega - \Omega'))}{1 + \tau_{12}/\tau_{21} + 2\tau_{12}|\Omega'|/\hbar}, \quad (25)$$

where $j = (N_2/N_1)(\tau_{12}/\tau_{21})$.

The system (25) is solved under the assumption that V_{rn} are small (weak coupling) and $\beta_c = (kT_c)^{-1}$ are large. We make use of the procedure developed in the papers of Bogolyubov [9]

and Zubarev and Tserkovnikov [10] for separating the principal terms that are logarithmic in β_c, obtaining

$$\chi_i = (V_{i1}N_1\chi_1 + V_{i2}N_2\chi_2)\ln\frac{2\gamma\beta}{\pi} + V_{i1}N_1\chi_1\ln\hbar\omega_{i1} + V_{i2}N_2\chi_2\ln\hbar\omega_{i2} + \frac{N_1(\chi_1-\chi_2)}{1+\tau_{12}/\tau_{21}}(V_{i2}j - V_{i1})I, \quad (26)$$

where $\chi_i = \chi_i(\delta)$, $V_{ij} = V_{ij}(\delta)$, $\delta \to 0$, $\gamma = e^C$, C is Euler's constant, and

$$I = \int_0^\infty \frac{dt}{t(1+t^2)}\,\mathrm{th}\left[\frac{\hbar\beta}{4\tau_{12}}\left(1+\frac{\tau_{12}}{\tau_{21}}\right)t\right]; \quad (27)$$

$$\ln\omega_{ij} = -\int_0^\infty \ln y\, d[(V_{ij}(\delta - iy) + V_{ij}(-\delta - iy))N_j(\chi_i(iy+\delta) + \chi_j(iy-\delta)][4V_{ij}N_j\chi_j]^{-1}. \quad (28)$$

The vanishing of the determinant of the system (26) defines the quantity β_c, and determines with it the critical temperature. The corresponding system of equations for the pure superconductor is obtained from (26) by dropping the terms containing I and replacing the frequencies ω_{ij} with the frequencies for the pure superconductor ω_{ij}^0. The corresponding determinant determines β_c^0. Let us expand the determinant of (26) in powers of I and of $\ln(\omega_{ij}/\omega_{ij}^0)$ and retain the linear terms. It is easy to see that the result is the following impurity dependence of β_c:

$$\ln\frac{\beta_c}{\beta_c^0} = A + B; \quad (29)$$

$$A = \frac{N_1 I}{D(1+\tau_{12}/\tau_{21})}\{(V_{22}j - V_{21})(1 - V_{11}N_1\xi_{11} - V_{12}N_2\xi_{12}) + (V_{12}j - V_{11})(V_{21}N_1\xi_{21} + V_{22}N_2\xi_{22} - 1), \quad (30)$$

$$B = -\frac{1}{D}\{V_{11}N_1\zeta_{11}(1 - V_{22}N_2\xi_{22}) + V_{22}N_2\zeta_{22}(1 - V_{11}N_1\xi_{11}) + V_{21}N_1V_{12}N_2(\zeta_{12}\xi_{21} + \zeta_{21}\xi_{12})\}, \quad (31)$$

$$D = V_{11}N_1(1 - V_{22}N_2\xi_{22}) + V_{22}N_2(1 - V_{11}N_1\xi_{11}) + V_{12}V_{21}N_1N_2(\xi_{21} + \xi_{12}); \quad (32)$$

$$\xi_{ij} = \ln\frac{2\gamma\beta_c^0\hbar\omega_{ij}}{\pi}, \qquad \zeta_{ij} = \ln\frac{\omega_{ij}}{\omega_{ij}^0}. \quad (33)$$

In the right side of (29) the principal term is A. Retaining in the latter only the terms that vanish when $V_{ij} \to 0$, we obtain

$$\xi = \ln\frac{2\gamma\beta_c^0\hbar\omega}{\pi} = \frac{b_0}{2a}\left[1 \pm \left(1 - \frac{4a}{b_0^2}\right)^{1/2}\right], \quad (34)$$

$$A = \mp N_1 I\Big\{V_{11} + V_{22}j - V_{21} - V_{12}j - \frac{N_1 j + N_2}{2N_1N_2}[b_0 \pm (b_0^2 - 4a)^{1/2}]\Big\} \times (1 + \tau_{12}/\tau_{21})^{-1}(b_0^2 - 4a)^{-1/2}, \quad (35)$$

$$b_0 = V_{11}N_1 + V_{22}N_2, \qquad a = N_1N_2(V_{11}V_{22} - V_{12}V_{21}), \quad (36)$$

where ω is some averaged frequency, introduced for convenience.

For spherically symmetrical Fermi-surface cavities j is equal to unity. In this case we have

$$\ln\frac{\beta_c}{\beta_c^0} \approx I\alpha^\pm = \alpha^\pm\left[\psi\left(\frac{1}{2} + \frac{\hbar\beta_c(1+\tau_{12}/\tau_{21})}{4\pi\tau_{12}}\right) - \psi\left(\frac{1}{2}\right)\right], \quad (37)$$

$$\alpha^\pm = \frac{1}{2}\Big\{1 \pm \Big[\frac{N_2 - N_1}{N_1 + N_2}(V_{22}N_2 - V_{11}N_1) + \frac{2N_1N_2}{N_1+N_2}(V_{12} + V_{21})\Big](b_0^2 - 4a)^{-1/2}\Big\}, \quad (38)$$

where ψ is the derivative of the logarithm of the Γ function.

In (34), (37), and (38) it is necessary to take the lower sign when $a \leq 0$, for otherwise we arrive at negative values of ξ. When $a > 0$ it is necessary to take the sign leading to a more stable superconducting state. Regardless of the choice of the sign, the values of α are not negative and do not exceed unity. This follows from the fact that the absolute value of the second term of the right side of (36) is always smaller than or equal to unity.

Formula (37) is similar to the Abrikosov and Gor'kov formula

$$\ln\frac{\beta_c}{\beta_c^0} = \psi\left(\frac{1}{2} + \frac{\beta_c}{2\pi\tau_s}\right) - \psi\left(\frac{1}{2}\right),$$

where τ_s is in this case the relaxation time of the spin interaction of the electron with the paramagnetic impurity.

In the limit of small impurity concentrations $\beta_c(1/\tau_{12} + 1/\tau_{21}) \ll 1$ we have

$$T_c \approx T_c^0 - \tfrac{1}{8}\pi\hbar\alpha^\pm(1/\tau_{12} + 1/\tau_{21}). \quad (39)$$

Thus, in the limit of low impurity concentration we observe a decrease in the critical temperature with increasing concentration.

Let us consider the second limiting case

$$\beta_c(1/\tau_{12} + 1/\tau_{21}) \gg 1. \quad (40)$$

To make this inequality compatible with (9) we must satisfy the condition

$$\mu\beta_c \gg \frac{m_2}{m_1}\frac{\beta_c}{2}\left(\frac{1}{\tau_{12}} + \frac{1}{\tau_{21}}\right) \gg 1. \quad (41)$$

In the limiting case (41), Eq. (37) with $\alpha^\pm \neq 1$

takes the form

$$\frac{\hbar\beta_c\gamma}{\pi}\left(\frac{1}{\tau_{12}}+\frac{1}{\tau_{21}}\right)=\left[\frac{\hbar\beta_c{}^0\gamma}{\pi}\left(\frac{1}{\tau_{12}}+\frac{1}{\tau_{21}}\right)\right]^{1/(1-\alpha^{\pm})}, \quad (42)$$

whereas for $\alpha^{\pm} = 1$ we have

$$\frac{1}{6}\left(\frac{2\pi}{\hbar\beta_c}\right)^2\left(\frac{1}{\tau_{12}}+\frac{1}{\tau_{21}}\right)^{-2}=\ln\left[\frac{\hbar\beta_c{}^0\gamma}{\pi}\left(\frac{1}{\tau_{12}}+\frac{1}{\tau_{21}}\right)\right]. \quad (43)$$

According to (43), $\beta \to \infty$ when

$$\hbar\beta_c{}^0(1/\tau_{12}+1/\tau_{21})\to 1,$$

that is, at some critical impurity concentration. When $\alpha^{\pm} \neq 1$, in accordance with (42), β_c can tend to infinity only if the impurity concentration increases without limit. This limiting case, obviously cannot be regarded by us. Thus, when $\alpha^{\pm} = 1$ there is no critical impurity concentration in this theory.

The results can be used when the d- and s-bands of transition metals overlap, and also when the s- and p-bands of metals of the principal groups of the periodic system overlap. For transitions metals, the d-band ($n = 2$) is much narrower than the s-band ($n = 1$), and inequality $N_2 \gg N_1$ holds. Since j is equal to unity, we also have the inequality

$$1/\tau_{12} \gg 1/\tau_{21},$$

making it possible to simplify the obtained formulas somewhat. Thus for example, (39) takes the form

$$\frac{\delta T_c}{T_c}\approx -\frac{\pi}{8}\alpha^{\pm}\frac{\hbar\beta_{c0}v_F}{l_{12}}, \qquad l_{12}=v_F\tau_{12}. \quad (44)$$

When $v_F/T_{c0} \sim 2 \times 10^7$ cm/sec-deg we have

$$\frac{\delta T_c}{T_c}\sim\frac{-6\cdot 10^{-5}\alpha^{\pm}[\text{cm}]}{l_{12}}.$$

The experimentally measured quantity is the transport mean free path $l = v_F\tau_{tr}$, and therefore

$$\frac{\delta T_c}{T_c}\sim\frac{6\cdot 10^{-5}\alpha^{\pm}(\tau_{tr}/\tau_{12})\ [\text{cm}]}{l}.$$

Since u_{1k} can be regarded as constant for the broad conduction band (s), whereas for the narrow (d) band u_{2k} varies rapidly near the ionic core, the quantity $\chi(1k, 2k')$ which is contained in the definition of τ_{12} is apparently small. This smallness is contained in quadratic fashion in the definition of the interband relaxation time. If we assume that the product of the two unknown parameters α and τ_{tr}/τ_{12} is of the order of 10^{-2}, then we obtain at low impurity concentrations

$$\frac{\delta T_c}{T_c}l\sim -10^{-6}\,\text{cm}.$$

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APPENDIX

We seek the solution of (19) in the form

$$K_{n_1n_2n_3n_4}(\mathbf{kk'}|\Omega\Omega')=\beta\delta_{\Omega\Omega'}\sum_{r_1r_2}\bar{G}_{n_1r_1}(\mathbf{k}|\Omega)\bar{G}_{n_2r_2}(-\mathbf{k}|-\Omega)\mathcal{H}_{r_1r_2n_3n_4}(\mathbf{kk'}|\Omega), \quad (A.1)$$

where the new function $\mathcal{H}$ satisfies the equation

$$\mathcal{H}_{r_1r_2n_3n_4}(kk'|\Omega)=\delta_{\mathbf{kk}'}\delta_{r_1n_3}\delta_{r_2n_4}+\frac{c}{V}\sum_{\mathbf{k}_1}|u(\mathbf{k}-\mathbf{k}_1)|^2$$
$$\times\sum_{\substack{m_1m_2\\ l_1l_2}}\chi(r_1\mathbf{k}m_1\mathbf{k}_1)\chi(r_2-\mathbf{k}m_2-\mathbf{k}_1)\bar{G}_{m_1l_1}(\mathbf{k}_1|\Omega)$$
$$\bar{G}_{m_2l_2}(-\mathbf{k}_1|-\Omega)\,\mathcal{H}_{l_1l_2n_3n_4}(\mathbf{k}_1\mathbf{k}'|\Omega). \quad (A.2)$$

On the basis of the properties of the functions $\tilde{G}$, given in Sec. 2, we can easily see that the product $\tilde{G}_{m_1l_1}\tilde{G}_{m_2l_2}$ is small when all the band indices coincide. Therefore, accurate to terms $\hbar m_2/2\tau_{ij}\mu m_1 \ll 1$ we can simplify (18) and (A.2) by retaining only the indicated essential terms. We then obtain

$$F_{nn'}(\mathbf{k}|\Omega)\approx\bar{G}_{nn}(\mathbf{k}|\Omega)\bar{G}_{n'n'}(-\mathbf{k}|-\Omega)\frac{1}{\beta V}$$
$$\times\sum_{\Omega'\mathbf{k}_1\mathbf{k}_2}\sum_{n_1\ldots n_4}B(\mathbf{k}_1-\mathbf{k}_2|\Omega-\Omega')$$
$$\times\mathcal{H}_{nn'n_1n_2}(\mathbf{kk}_1|\Omega)\chi(n\mathbf{k}_1n_3\mathbf{k}_2)\chi(n_2-\mathbf{k}_1n_4-\mathbf{k}_1)$$
$$\times F_{n_3n_4}(\mathbf{k}_2|\Omega'), \quad (A.3)$$

$$\mathcal{H}_{nn'n_1n_2}(\mathbf{kk}_1|\Omega)\approx\delta_{\mathbf{kk}_1}\delta_{nn_1}\delta_{n'n_2}+\frac{c}{V}\sum_{\mathbf{k}_2}|u(\mathbf{k}-\mathbf{k}_2)|^2$$
$$\times\sum_{m}\chi(n\mathbf{k}m\mathbf{k}_2)\chi^*(n'\mathbf{k}m\mathbf{k}_2)\bar{G}_{mm}(\mathbf{k}_2|\Omega)$$
$$\times G_{mm}(-\mathbf{k}_2|-\Omega)\mathcal{H}_{mmn_1n_2}(\mathbf{k}_2\mathbf{k}_1|\Omega). \quad (A.4)$$

It is convenient to make in (A.3) the substitution

$$F_{nn'}(\mathbf{k}|\Omega)=G_{nn}(\mathbf{k}|\Omega)G_{n'n'}(-\mathbf{k}|-\Omega)f_{nn'}(\mathbf{k}|\Omega). \quad (A.5)$$

We then obtain for the function $f_{nn'}$

$$f_{nn'}(\mathbf{k}|\Omega)\approx\frac{1}{\beta V}\sum_{\substack{\Omega'n_1n_2n_3\\ \mathbf{k}_1\mathbf{k}_3}}\sum B(\mathbf{k}_1-\mathbf{k}_2|\Omega-\Omega')$$
$$\times\mathcal{H}_{nn'n_1n_2}(\mathbf{kk}_1|\Omega)\chi(n_1\mathbf{k}_1n_3\mathbf{k}_2)\chi^*(n_2\mathbf{k}n_3\mathbf{k}_2)$$
$$\times\bar{G}_{n_3n_3}(\mathbf{k}_2|\Omega')\bar{G}_{n_3n_3}(-\mathbf{k}_2|-\Omega')f_{n_3n_3}(\mathbf{k}_3|\Omega'). \quad (A.6)$$

From this equation it follows that the off-diagonal

elements of the function $f_{nn'}$ ($n \neq n'$) depend linearly on the diagonal elements ($n = n'$) and by the same token the critical temperature T_c of the superconductor (and with it also $\beta = \beta_c$) is determined from the system of two equations (A.6) for the function $f_n(\mathbf{k}|\Omega)$.

Using the property

$$\mathcal{H}_{nn\,n_1n_2}(\mathbf{k}\mathbf{k}'|\Omega) = \delta_{n_1n_2}\mathcal{H}_{nn\,n_1n_1}(\mathbf{k}\mathbf{k}'|\Omega), \quad (A.7)$$

which follows from (A.4) we obtain for the functions $f_{nn}(\mathbf{k}|\Omega)$ the system of equations ($\beta = \beta_c$):

$$f_{nn}(\mathbf{k}|\Omega) = \frac{1}{\beta V}\sum_{\Omega'}\sum_{rm}\sum_{\mathbf{k}_1\mathbf{k}_2} B(\mathbf{k}_1-\mathbf{k}_2|\Omega-\Omega')\mathcal{H}_{nnrr}(\mathbf{k}\mathbf{k}_1|\Omega)$$
$$\times|\chi(r\mathbf{k}_1\, m\mathbf{k}_2)|^2 G_{mm}(\mathbf{k}_2|\Omega')\bar{G}_{mm}(-\mathbf{k}_2|-\Omega')f_{mm}(\mathbf{k}_2|\Omega'). \quad (A.8)$$

We introduce, finally, a new function

$$L_{rm}(\mathbf{k}\mathbf{k}_1|\Omega\Omega') = \sum_{n\mathbf{k}_2}\mathcal{H}_{rrnn}(\mathbf{k}\mathbf{k}_2|\Omega)|\chi(n\mathbf{k}_2\, m\mathbf{k}_1)|^2$$
$$\times B(\mathbf{k}_2-\mathbf{k}_1|\Omega-\Omega'). \quad (A.9)$$

We then obtain the system of equations

$$f_{rr}(\mathbf{k}|\Omega) = \frac{1}{\beta V}\sum_{\mathbf{k},\Omega'}\sum_{m} L_{rm}(\mathbf{k}\mathbf{k}_1|\Omega\Omega')\bar{G}_{mm}(\mathbf{k}_1|\Omega')$$
$$\times \bar{G}_{mm}(-\mathbf{k}_1|-\Omega')f_{mm}(\mathbf{k}_1|\Omega'), \quad (A.10)$$

$$L_{rm}(\mathbf{k}\mathbf{k}'|\Omega\Omega') = B(\mathbf{k}-\mathbf{k}'|\Omega-\Omega')|\chi(r\mathbf{k}\, m\mathbf{k}')|^2$$
$$+\frac{c}{V}\sum_{\mathbf{p}n}|u(\mathbf{k}-\mathbf{p})|^2|\chi(r\mathbf{k}\, n\mathbf{p})|^2\bar{G}_{nn}(\mathbf{p}|\Omega)$$
$$\times\bar{G}_{nn}(-\mathbf{p}|-\Omega)L_{nm}(\mathbf{p}\mathbf{k}'|\Omega\Omega'). \quad (A.11)$$

We solve it by using the rapid decrease of the product of two Green's functions with increasing distance from the Fermi surface, so that the functions f and L need be considered only on the Fermi surface

$$f_{rr}(\mathbf{k}_r{}^F|\Omega) \approx \frac{1}{\beta}\sum_{\Omega'}\sum_{m}\frac{\pi}{(2\pi\hbar)^3}\int_{S_m}\frac{dS_m}{|\nabla E_m|}L_{rm}(\mathbf{k}_r{}^F\mathbf{p}_m{}^F|\Omega\Omega')$$
$$\times\Lambda_m(\Omega')f_{mm}(\mathbf{p}_m{}^F|\Omega'), \quad (A.12)$$

$$\Lambda_m(\Omega) = \frac{1}{\pi}\int_{E_m^{min}}^{E_m^{max}} G_{mm}(\mathbf{k}|\Omega)G_{mm}(-\mathbf{k}|-\Omega)\,dE_m$$
$$= \frac{1}{|\Omega|\eta_m(\Omega)}. \quad (A.13)$$

Furthermore

$$\int_{S_m} L_{rm}(\mathbf{k}_r{}^F\mathbf{g}_m{}^F|\Omega\Omega')\frac{dS_m}{|\nabla E_m|}$$
$$= \int_{S_m}\frac{dS_m}{|\nabla E_m|}B(\mathbf{k}\mathbf{r}^F-\mathbf{g}_m{}^F|\Omega-\Omega')|\chi(r\mathbf{k}_r{}^F\, m\mathbf{g}_m{}^F)|^2$$
$$+\frac{c\pi}{(2\pi\hbar)^3}\sum_n\int_{S_n}\frac{dS_n}{|\nabla E_n|}|u(\mathbf{k}_L{}^F-\mathbf{p}_n{}^F)|^2|\chi(r\mathbf{k}_r{}^F\, n\mathbf{p}_n{}^F)|^2$$
$$\times\Lambda_n(\Omega)\int_{S_m}\frac{dS_m}{|\nabla E_m|}L_{nm}(\mathbf{p}_n{}^F\mathbf{g}_m{}^F|\Omega\Omega'). \quad (A.14)$$

We introduce the notation

$$(2\pi)^3V_{rm}(\Omega-\Omega')N_m = \int_{S_m}\frac{dS_m}{|\nabla E_m|}B(k_r{}^F-g_m{}^F|\Omega-\Omega')$$
$$\times|\chi(rk_r{}^F\, mg_m{}^F)|^2,$$

$$2\pi^2L_{rm}(\Omega\Omega')N_m = \int_{S_m}\frac{dS_m}{|\nabla E_m|}L_{rm}(k_r{}^Fg_m{}^F|\Omega\Omega'), \quad (A.15)$$

where

$$N_m = \frac{1}{2\pi^2}\left|\frac{k^2}{\nabla E_m}\right|_{k_m^F} \quad (A.16)$$

is the state density on the m-th cavity of the Fermi surface. Just as for the relaxation times τ_{ij}, we assume here that the quantities V_{rm}, L_{rm}, and f_{rr} are independent of the orientation of the vector $\mathbf{k}_r^F$, the end point of which lies on the r-th cavity of the Fermi surface. Whenever this assumption does not hold, the theory becomes essentially anisotropic.

Thus, the isotropic theory is based on the following equations ($f_r(\Omega) = f_{rr}(\mathbf{k}_{rr}F|\Omega)$):

$$f_r(\Omega) \approx \frac{1}{4\beta}\sum_{\Omega'}\sum_{m}L_{rm}(\Omega\Omega')N_m\Lambda_m(\Omega')f_m(\Omega'), \quad (A.17)$$

$$L_{rm}(\Omega\Omega') = 4\pi V_{rm}(\Omega-\Omega') + \sum_n\frac{\hbar}{2\tau_{rn}}L_{nm}(\Omega\Omega'). \quad (A.18)$$

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