EFFECT OF IMPURITIES ON THE SUPERCONDUCTING TRANSITION TEMPERATURE

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The effect of diamagnetic impurities on the superconducting transition temperature is considered for that case when, by the addition of impurities, it is possible to modify the topology of the superconductor's Fermi surface. It is shown that under these conditions the dependence of the superconducting transition temperature on the impurity concentration n is nonlinear ($T_k \sim \sqrt{n} \ln n$). Depending on the nature of the change in the topology of the Fermi surface, the superconducting transition temperature T_k may both increase and decrease with increasing n.

1. A large amount of experimental data on the effect of nonmagnetic impurities on the superconducting transition temperature was satisfactorily explained by Kadanoff and Markowitz,[1] and also by Hohenberg.[2] In order to explain the nonlinear change of the superconducting transition temperature T_k with increase of the impurity concentration, Kadanoff and Markowitz considered a superconductor with an anisotropic potential for the electron-electron interaction. It was shown that owing to the anisotropy of the electron-electron interaction the superconducting transition temperature decreases with increasing impurity concentration, reaching some limiting value for $\omega_D\tau \gg 1$, where ω_D is the Debye temperature and τ is the time of free flight of the electrons, determined by the scattering of the electrons by impurities. However, this theory does not explain the nonlinear increase of T_k with increase of the impurity concentration for thallium.[3] In a series of articles,[4-6] it was shown that the nonlinear increase in the superconducting transition temperature of thallium with pressure can be related to a change in the topology of the thallium Fermi surface under pressure.

In the present article we investigate the nonlinear change of T_k, caused by a change in the topology of the Fermi surface under the influence of impurities. Among the superconductors for which a modification of the topology of the Fermi surface is possible under the influence of impurities, besides thallium, are apparently the metals having small groups of electrons (Zn, Ga, In, etc.) or metals in which magnetic breakdown is observed (Zn). A combined account of anisotropy of the electron-electron interaction and of the singularities associated with a change in the topology of the Fermi surface appreciably complicates the investigation of the effect of impurities on T_k. We assume that the anisotropy of the electron-electron interaction is small (as is the case for a number of superconductors[1]), and consider only the nonlinear change of T_k under the influence of impurities, due to modification of the topology of the Fermi surface. We shall show that this mechanism, in contrast to that considered by Kadanoff and Markowitz, may lead to both a nonlinear decrease and to a nonlinear increase of T_k with increasing concentration of impurities.

2. In order to take account of the effect of impurities on the superconducting transition temperature T_k and on the energy gap Δ in that case when the density of electron states $\nu(\varepsilon)$ has singularities associated with a change in the topology of the Fermi surface,[7] it is necessary to consider the system of equations for the Green's functions of the superconductor. We represent the effective Hamiltonian of the electron-electron interaction in the form[8]

$$H^{(e)} = -\frac{1}{2}\int \lambda\psi^+(\mathbf{r})\psi^+(\mathbf{r})\psi(\mathbf{r})\psi(\mathbf{r})\,d\mathbf{r}, \qquad (1)$$

where λ is the effective potential of the electron-electron interaction, and ψ^+ and ψ are the electron creation and annihilation operators in the representation of second quantization. As is customary, we describe the interaction of electrons with impurities by the Hamiltonian

$$H^{(i)} = \int \psi^+(\mathbf{r})\hat{V}(\mathbf{r})\psi(\mathbf{r})\,d\mathbf{r}, \qquad \hat{V} = \sum_j v(\mathbf{r}-\mathbf{r}_j), \qquad (2)$$

where $v(\mathbf{r} - \mathbf{r}_j)$ is the potential for the interaction of an electron with the j-th impurity atom and the summation over j denotes a summation over all impurity atoms.

We shall derive the system of equations for the Green's functions by following the work of Kadanoff and one of the authors.[9] The one-electron Green's function is defined in the following manner:

$$G_{\alpha\beta}(\mathbf{r}_1 t_1;\ \mathbf{r}_1' t_1') \equiv G_{\alpha\beta}(1, 1') = -i\langle T\psi_\alpha(\mathbf{r}_1 t_1)\psi_\beta^+(\mathbf{r}_1' t_1')\rangle, \tag{3}$$

where the angle brackets denote statistical averaging and T is the time-ordering operator.

In order to obtain an equation for the Green's function $G_{\alpha\beta}(1, 1')$, we differentiate it with respect to its first time argument, and we use the equation of motion for Heisenberg operators[16]

$$i\partial\psi_\alpha(\mathbf{r}, t)\,/\,\partial t = [\psi_\alpha(\mathbf{r}, t), \quad H - N\mu]. \tag{4}$$

Here we obtain a term representing the average of the product of four ψ-operators. Following well known methods,[10] we decompose it into an average of products of the two operators $\psi(\mathbf{r}, t)$ and $\psi^+(\mathbf{r}, t)$. Upon making such a separation, new one-electron Green's functions appear:

$$\begin{aligned} F_{\alpha\beta}(1, 1') &= -i\langle T\psi_\alpha(1)\psi_\beta(1')\rangle, \\ F_{\alpha\beta}^+(1, 1') &= -i\langle T\psi_\alpha^+(1)\psi_\beta^+(1')\rangle, \\ G_{\alpha\beta}^{tr}(1, 1') &= -i\langle T\psi_\beta(1')\psi_\alpha^+(1)\rangle. \end{aligned} \tag{5}$$

The equations of motion for these Green's functions are obtained according to the same scheme as the equation of motion for the Green's function $G_{\alpha\beta}(1, 1')$. As a result, we obtain a system of four equations for the four one-electron Green's functions. This system may be symbolically written in matrix form:[11]

$$\begin{pmatrix} i\dfrac{\partial}{\partial t_1} + \dfrac{\Delta_1}{2m} + \mu - \hat{V}(1) - i\lambda G(1, 1) & -\dfrac{\lambda}{i}F(1,1) \\ -\dfrac{\lambda}{i}F^+(1, 1) & i\dfrac{\partial}{\partial t_1} - \dfrac{\Delta_1}{2m} - \mu + \hat{V}(1) - i\lambda G^{tr}(1, 1) \end{pmatrix}$$

$$\times \begin{pmatrix} \hat{G}(1, 1') & \hat{F}(1, 1') \\ \hat{F}^+(1, 1') & -\hat{G}^{tr}(1, 1') \end{pmatrix}$$

$$= \begin{pmatrix} \delta(1-1') & 0 \\ 0 & \delta(1-1') \end{pmatrix}. \tag{6}$$

Such a symbolic notation enables us to call attention to the fact that the four one-electron Green's functions $\hat{G}$, $\hat{F}$, $\hat{F}^+$, and G^{tr} form a single four-row matrix Green's function:

$$g_{\alpha\beta}(1, 1') = \begin{pmatrix} \hat{G}(1, 1') & \hat{F}(1, 1') \\ \hat{F}^+(1, 1') & -\hat{G}^{tr}(1, 1') \end{pmatrix}$$

$$= -i\langle T\Psi_\alpha(1)\Psi_\beta^+(1')\rangle, \tag{7}$$

where $\alpha, \beta = 1, 2, 3, 4$; ψ_α and ψ_β^+ are new four component creation and annihilation operators:[12, 13]

$$\Psi(1) = \begin{pmatrix} \psi_\uparrow(1) \\ \psi_\downarrow(1) \\ \psi_\uparrow^+(1) \\ \psi_\downarrow^+(1) \end{pmatrix},$$

$$\Psi^+(1) = (\psi_\uparrow^+(1),\ \ \psi_\downarrow^+(1),\ \ \psi_\uparrow(1),\ \ \psi_\downarrow(1)). \tag{8}$$

Use of (8) and the four-row matrices

$$\hat{\tau}_1 = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}, \quad \hat{\sigma}_2 = i\begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{pmatrix},$$

$$\hat{\tau}_3 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}, \quad \hat{I} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \tag{9}$$

enables us to rewrite Eq. (6) in the form of a single equation:[6]

$$\hat{L}\hat{g}(1, 1') - \hat{V}(1)\,\hat{\tau}_3\hat{g}(1, 1') = \delta(1-1'),$$

$$\hat{L} = \left[i\frac{\partial}{\partial t_1}\hat{I} + \left(\frac{\Delta_1}{2m} + \mu\right)\hat{\tau}_3 - i\lambda\hat{\tau}_3\hat{g}(1, 1)\,\hat{\tau}_3\right]. \tag{10}$$

We must average over the positions of the impurities, which are assumed to be randomly distributed. On the left side of Eq. (10) there is only one term with $\hat{V}(1)$, besides the Green's function $\hat{g}(1, 1')$, depending on the positions of the impurities. The same operation of averaging over the impurity positions pertains to the product $\hat{V}(1)\ \hat{\tau}_3\hat{g}(1, 1')$. In order to accomplish this averaging, we introduce a new function $\hat{\Sigma}(1, 1')$, with the aid of which we write the average, over the positions of the impurities, of the product in the following way:[1)]

$$\langle\hat{V}(1)\ \hat{\tau}_3\hat{g}(1, 1')\rangle_{imp} = \int_0^{(iT)^{-1}} dt_2 \int d\mathbf{r}_2\, \hat{\Sigma}(1',2)\,\langle\hat{g}(2, 1')\rangle_{imp}, \tag{11}$$

where the angle brackets with the subscript imp denote averaging over the positions of the impurities. Therefore, after averaging one can represent Eq. (10) in the form

$$\hat{L}\,\langle\hat{g}(1-1')\rangle_{imp} - \int d2\,\hat{\Sigma}(1, 2)\,\langle\hat{g}(2-1')\rangle_{imp} = \delta(1-1'). \tag{12}$$

Taking the well known relation

$$\int d2\,\hat{g}^{-1}(1, 2)\,\hat{g}(2, 1') = \delta(1-1')$$

into account, after multiplying Eq. (12) by $\hat{g}^{-1}(1, 2)$

[1)] Such an approximation is similar to that employed in other articles.[14,15]

and integrating over the 2 variable, we obtain an equation for $\hat{g}^{-1}(1, 2)$:

$$\langle \hat{g}^{-1}(1,2)\rangle_{imp} = \left\{ i\frac{\partial}{\partial t_1} + \left(\frac{\Delta_1}{2m} + \mu\right)\hat{\tau}_3 \right\}\delta(1-2)$$

$$-\hat{\Delta}(1)\delta(1-2) - \hat{\Sigma}(1, 2) \tag{13}$$

$$\hat{\Delta} = -i\lambda\hat{\tau}_3\hat{g}(1, 1)\hat{\tau}_3. \tag{14}$$

An unknown function $\hat{\Sigma}(1, 2)$, describing the interaction of electrons with impurity atoms, enters into Eq. (13). In order to determine it, we represent the Green's function $\hat{g}(1, 1')$ in the form of an expansion in powers of the potential for the interaction with impurities:

$$\hat{g}(1, 1') = \hat{g}^0(1-1') + \hat{g}^{(1)}(1, 1') + \ldots$$

The functions $\hat{g}^0(1-1')$ and $\hat{g}^{(1)}(1, 1')$, as one can easily see from Eq. (10), satisfy the equations

$$\hat{L}\hat{g}^0(1-1') = \delta(1-1'),\quad \hat{L}\hat{g}^{(1)}(1, 1') = \hat{V}(1)\hat{\tau}_3\hat{g}^0(1-1').$$

Hence

$$\hat{g}^{(1)}(1, 1') = \int d2\,\hat{g}^0(1-2)\hat{V}(2)\ \ g^0(2-1').$$

Using this expression for $\hat{g}^{(1)}(1, 1')$ and considering that $\langle\hat{V}\rangle = 0$, from (11) it is easy to find that, correct to terms of second order in the potential $\hat{V}$, the quantity $\hat{\Sigma}$ is given by

$$\hat{\Sigma}(1, 2) = \langle\hat{V}(1)\hat{\tau}_3\langle\hat{g}(1-2)\rangle_{imp}\hat{V}(2)\hat{\tau}_3\rangle_{imp}.$$

In order to simplify the calculations, we assume a point interaction between electron and impurities:

$$\hat{V}(1) = \sum_j v\delta(\mathbf{r}-\mathbf{r}_j). \tag{15}$$

As a result of averaging over the positions of the impurities, with the use of relations (15) we obtain:

$$\hat{\Sigma}(1, 1') = nv^2\hat{\tau}_3\langle\hat{g}(1-1')\rangle_{imp}\hat{\tau}_3\delta(\mathbf{r}_1-\mathbf{r}_1'), \tag{16}$$

where n is the number of impurity atoms (in order to simplify the notation, in what follows we shall omit the symbol indicating averaging over impurities).

Now let us go over to the Fourier components of the Green's function $\hat{g}(1-1')$ according to the formula

$$\hat{g}(1-1') = iT\sum_\nu\int\frac{d\mathbf{p}}{(2\pi)^3}\hat{g}_\nu(\mathbf{p})$$

$$\times\exp\left[i(\mathbf{p}, \mathbf{r}-\mathbf{r}') - i\zeta_\nu(t-t')\right], \tag{17}$$

where $\zeta_\nu = i\pi\nu T$ and the summation is over all odd integers ν. Using (15) and (17), we write Eq. (12) in the form

$$[\hat{g}_\nu(\mathbf{p})]^{-1} = \zeta_\nu\hat{I} - \varepsilon_{\mathbf{p}}\hat{\tau}_3 - \hat{\Delta} - nv^2\hat{\tau}_3\int\frac{d\mathbf{p}}{(2\pi)^3}\hat{g}_\nu(\mathbf{p})\hat{\tau}_3, \tag{18}$$

$$\hat{\Delta} = \lambda T\sum_\nu\int\frac{d\mathbf{p}}{(2\pi)^3}\hat{\tau}_3\hat{g}_\nu(\mathbf{p})\hat{\tau}_3, \tag{19}$$

where the energy $\varepsilon_{\mathbf{p}}$ is measured from the chemical potential μ.

In order to solve Eq. (18), we use a representation of the Green's function $[\hat{g}_\nu(\mathbf{p})]^{-1}$ in the form of a sum of terms, each of which has a definite matrix structure. Two obvious terms are the terms proportional to the unit matrix $\hat{I}$ and to the matrix $\hat{\tau}_3$, since such terms already explicitly occur in Eq. (18). The form of the remaining terms is determined from the structure of the operator Δ. Using relations (5), (7), and (14), one can show that

$$\hat{\Delta} = \Delta\cdot\hat{\tau}_1\hat{\sigma}_2, \tag{20}$$

where $\Delta = \lambda F(1, 1)$ is a real quantity (here we omit the term $\hat{G}(1, 1)\hat{\tau}_3$ since it may be included in the renormalization of the chemical potential).

Thus, in the expression for $[\hat{g}_\nu(\mathbf{p})]^{-1}$ there will be one more term, proportional to the matrix $\hat{\tau}_1\hat{\sigma}_2$. Therefore, the function $\hat{g}^{-1}(\mathbf{p})$ is written in the following matrix form

$$[\hat{g}_\nu(\mathbf{p})]^{-1} = \tilde{\omega}(\zeta_\nu)\hat{I} - \tilde{\varepsilon}_{\mathbf{p}}(\zeta_\nu)\hat{\tau}_3 - \tilde{\Delta}(\zeta_\nu)\hat{\tau}_1\hat{\sigma}_2 \tag{21}$$

with the functions $\tilde{\omega}(\zeta_\nu)$, $\tilde{\varepsilon}_{\mathbf{p}}(\zeta_\nu)$, and $\tilde{\Delta}(\zeta_\nu)$ subject to determination. A system of three equations for these functions is found by substitution of expression (21) into Eq. (18), and by setting them equal to the terms in front of the matrices $\hat{I}$, $\hat{\tau}_3$, and $\hat{\tau}_1\hat{\sigma}_2$, respectively.

$$\tilde{\omega}(\zeta_\nu) = \zeta_\nu - nv^2\tilde{\omega}(\zeta_\nu)\int\frac{d\mathbf{p}}{(2\pi)^3}\frac{1}{\tilde{\omega}^2(\zeta_\nu) - \tilde{\varepsilon}_{\mathbf{p}}^2(\zeta_\nu) - \tilde{\Delta}^2(\zeta_\nu)}, \tag{22}$$

$$\tilde{\varepsilon}_{\mathbf{p}}(\zeta_\nu) = \varepsilon_{\mathbf{p}} + nv^2\int\frac{d\mathbf{p}}{(2\pi)^3}\frac{\tilde{\varepsilon}_{\mathbf{p}}(\zeta_\nu)}{\tilde{\omega}^2(\zeta_\nu) - \tilde{\varepsilon}_{\mathbf{p}}^2(\zeta_\nu) - \tilde{\Delta}^2(\zeta_\nu)}, \tag{23}$$

$$\tilde{\Delta}(\zeta_\nu) = \Delta - nv^2\tilde{\Delta}(\zeta_\nu)\int\frac{d\mathbf{p}}{(2\pi)^3}\frac{1}{\tilde{\omega}^2(\zeta_\nu) - \tilde{\varepsilon}_{\mathbf{p}}^2(\zeta_\nu) - \tilde{\Delta}^2(\zeta_\nu)}. \tag{24}$$

The equation for the superconductor's gap is obtained from (19) and (20):

$$\Delta = -\lambda T\sum_\nu\int\frac{d\mathbf{p}}{(2\pi)^3}\frac{\tilde{\Delta}(\zeta_\nu)}{\tilde{\omega}^2(\zeta_\nu) - \tilde{\varepsilon}_{\mathbf{p}}^2(\zeta_\nu) - \tilde{\Delta}^2(\zeta_\nu)}. \tag{25}$$

After substituting $\tilde{\Delta}(\zeta_\nu)$ from (24) and cancellation of the quantity Δ, this equation is rewritten in the following way:

$$1 = -\lambda T\sum_\nu\int\frac{d\mathbf{p}}{(2\pi)^3}[\tilde{\omega}^2(\zeta_\nu) - \tilde{\varepsilon}_{\mathbf{p}}^2(\zeta_\nu) - \tilde{\Delta}^2(\zeta_\nu)]^{-1}$$

$$\times\left\{1 + nv^2\int\frac{d\mathbf{p}}{(2\pi)^3}[\tilde{\omega}^2(\zeta_\nu) - \tilde{\varepsilon}_{\mathbf{p}}^2(\zeta_\nu) - \tilde{\Delta}^2(\zeta_\nu)]^{-1}\right\}^{-1}. \tag{26}$$

Since we are interested in the question of the superconducting transition temperature, then in

Eq. (26) we assume $\tilde{\Delta}(\zeta_\nu) = 0$, by the same token obtaining an equation for T_k:

$$1 = \lambda T_k \sum_\nu \int \frac{d\mathbf{p}}{(2\pi)^3} [\tilde{\omega}^2(\zeta_\nu) - \tilde{\varepsilon}_\mathbf{p}^2(\zeta_\nu)]^{-1}$$
$$\times \left\{1 + nv^2 \int \frac{d\mathbf{p}}{(2\pi)^3} [\tilde{\omega}^2(\zeta_\nu) - \tilde{\varepsilon}_\mathbf{p}^2(\zeta_\nu)]^{-1}\right\}^{-1}. \tag{27}$$

Taking the dependence of the integrands in formulas (22)–(27) on the electron energy into consideration, it is convenient to change from integration over momentum to integration over energy:

$$d\mathbf{p} / (2\pi)^3 = \nu(\varepsilon)\, d\varepsilon,$$

by introducing in the usual way the density of normal single-particle states:[17]

$$\nu(\varepsilon) = \frac{1}{(2\pi)^3} \int \frac{dS}{v_F},$$

where $v_F = \partial\varepsilon/\partial p$ is the electron velocity on the equal-energy surface $\varepsilon(\mathbf{p}) = \mathrm{const}$ and dS is an infinitesimal element of this surface. As was shown by I. M. Lifshitz,[7] the quantity $\nu(\varepsilon)$ has a singularity near those values of the energy where the nature of the topology of the Fermi surface is modified and may be represented in the form

$$\nu(\varepsilon) = \nu_0(\varepsilon) + \delta\nu(\varepsilon),$$

where $\nu_0(\varepsilon)$ is a smooth function of the electron energy, and $\delta\nu(\varepsilon)$ is some nonmonotonic correction which is usually small in comparison with $\nu_0(\varepsilon)$.

Since in Eqs. (22)–(24), defining the functions $\tilde{\omega}$, $\tilde{\varepsilon}_\mathbf{p}$, and $\tilde{\Delta}$, the concentration of impurity atoms stands in front of the integrals, it is sufficient to consider in them only the smooth part $\nu_0(\varepsilon)$ of the density of states, evaluated for $\varepsilon = \varepsilon_F$. As a result, the basic system is written in the form

$$\Delta = -\lambda T \sum_\nu \int_{-\omega_D}^{+\omega_D} d\varepsilon_\mathbf{p} \frac{\nu(\varepsilon + \varepsilon_F)\tilde{\Delta}(\zeta_\nu)}{\tilde{\omega}^2(\zeta_\nu) - \varepsilon_\mathbf{p}^2 - \tilde{\Delta}^2(\zeta_\nu)}, \tag{28}$$

$$\tilde{\Delta}(\zeta_\nu) = \Delta - \frac{\Gamma}{2\pi}\tilde{\Delta}(\zeta_\nu) \int_{-\omega_D}^{+\omega_D} \frac{d\varepsilon_\mathbf{p}}{\tilde{\omega}^2(\zeta_\nu) - \varepsilon_\mathbf{p}^2 - \tilde{\Delta}^2(\zeta_\nu)}, \tag{29}$$

$$\tilde{\varepsilon}_\mathbf{p}(\zeta_\nu) = \varepsilon_\mathbf{p}, \tag{30}$$

$$\tilde{\omega}(\zeta_\nu) = \zeta_\nu - \frac{\Gamma}{2\pi}\tilde{\omega}(\zeta_\nu) \int_{-\omega_D}^{+\omega_D} \frac{d\varepsilon_\mathbf{p}}{\tilde{\omega}^2(\zeta_\nu) - \varepsilon_\mathbf{p}^2 - \tilde{\Delta}^2(\zeta_\nu)}, \tag{31}$$

where $\Gamma = 2\pi v^2 \nu_0(\varepsilon_F)n$ is the number of collisions of an electron with impurity atoms. A cut-off in the electron energy has been introduced in the integrals.[18, 19]

At the superconducting transition temperature $\Delta = \tilde{\Delta} = 0$, and from Eq. (31) we find that

$$\tilde{\omega}(\zeta_\nu) = \zeta_\nu + i\frac{\Gamma}{2}\,\mathrm{sign}\,\mathrm{Im}\,\zeta_\nu. \tag{32}$$

Recognizing that $\tilde{\varepsilon} = \varepsilon$, one can perform the integration over ε in the second factor in formula (27). Since in this factor the impurity concentration stands in front of the integral over ε, we shall not consider in the integration the nonmonotonic part $\delta\nu$ of the density of electron states:

$$nv^2 \int \frac{d^3\mathbf{p}}{(2\pi)^3} [\tilde{\omega}^2(\zeta_\nu) - \varepsilon_\mathbf{p}^2(\zeta_\nu)]^{-1}$$
$$\cong -\frac{\Gamma}{2}\,\frac{\mathrm{sign}\,\mathrm{Im}\,\zeta_\nu}{\pi\nu T_k + {}^1/{}_2\Gamma\,\mathrm{sign}\,\mathrm{Im}\,\zeta_\nu}.$$

Substituting this expression into (27) and changing from summation over all odd numbers ν to summation over all positive odd numbers, we obtain

$$1 = 2\lambda T_k \int_{-\omega_D}^{+\omega_D} d\varepsilon\, \nu(\varepsilon + \varepsilon_F) \sum_{\nu=1}^{\infty} \frac{\pi\nu T_k + \Gamma/2}{\pi\nu T_k}$$
$$\times \frac{1}{(\pi\nu T_k + \Gamma/2)^2 + \varepsilon^2}. \tag{33}$$

In this equation it is convenient to change from a summation over ν to an integration over ω. Using the formula[20]

$$T \sum_\nu h(\zeta_\nu) = \frac{1}{2\pi}\,\mathrm{Im} \int_0^\infty d\omega\, h(\omega)\,\mathrm{th}\frac{\omega}{2T},$$

we obtain*

$$1 = -\lambda\,\mathrm{Im} \int_0^\infty \frac{d\omega}{\pi} \int_{-\omega_D}^{+\omega_D} d\varepsilon\,\mathrm{th}\frac{\omega}{2T_k}\nu(\varepsilon + \varepsilon_F)$$
$$\times \frac{\omega + i\Gamma/2}{\omega[(\omega + i\Gamma/2)^2 - \varepsilon^2]}. \tag{34}$$

3. Equation (34) is the initial equation for investigating the dependence of the superconducting transition temperature on the concentration of impurity atoms. In order to evaluate the dependence of T_k on Γ, it is necessary to take the dependence of ε_F on the impurity concentration into consideration. We shall consider this dependence in the following manner:

$$\varepsilon_F = \varepsilon_F^0 + \alpha\Delta z\Gamma, \tag{35}$$

where ε_F^0 is the Fermi energy in a pure metal, Δz is the difference between the valences of the impurity atoms and the metal atoms, and α is some numerical coefficient.

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*th ≡ tanh.

In order to obtain a specific expression for T_k, it is necessary to know the nonmonotonic part of the density of electron states. As found in the article by Lifshitz,[7] $\delta\nu$ has the form

$$\delta\nu(\varepsilon) = \begin{cases} \mp \dfrac{m_1}{2\pi^2}[2m_3(\varepsilon_k - \varepsilon)]^{1/2}\theta(\varepsilon_k - \varepsilon) \\ \mp \dfrac{m_1}{2\pi^2}[2m_3(\varepsilon - \varepsilon_k)]^{1/2}\theta(\varepsilon - \varepsilon_k) \end{cases} . \qquad (36)$$

The upper line on the right side of formula (36) corresponds to the case of transition from a closed Fermi surface to an open one or to the disappearance of a group of electrons, and the lower line corresponds to the case of a transition from an open Fermi surface to a closed one or to the appearance of a new group of electrons. The minus sign refers to transitions from an open to a closed Fermi surface, and the plus sign refers to the appearance or disappearance of a specific group of electrons.

Let us consider first the case of the appearance of an electron group. In this case

$$\delta\nu(\varepsilon) = A\sqrt{\varepsilon - \varepsilon_k}\,\theta(\varepsilon - \varepsilon_k),$$

where $A = m_1\sqrt{2m_3}/2\pi^2$ and $\theta(x)$ is equal to unity for positive values of the argument and zero for negative values. For the case being analyzed, that of the appearance of an electron group in the equation for T_k, $\nu(\varepsilon + \varepsilon_F)$ is to be understood as the following quantity:

$$\begin{aligned} \nu(\varepsilon + \varepsilon_F) &= \nu_0(\varepsilon + \varepsilon_F{}^0 + \alpha\Delta z\Gamma) \\ &\quad + A(\varepsilon + \varepsilon_F{}^0 + \alpha\Delta z\Gamma - \varepsilon_k)^{1/2} \\ &\quad \times \theta(\varepsilon + \varepsilon_F{}^0 + \alpha\Delta z\Gamma - \varepsilon_k). \end{aligned} \qquad (37)$$

Using expression (37), let us rewrite Eq. (34) in the form

$$\begin{aligned} 1 = &-\lambda\,\mathrm{Im}\int_0^\infty \frac{d\omega}{\pi}\int_{-\omega_D}^{+\omega_D} d\varepsilon\,\mathrm{th}\frac{\omega}{2T_k}\nu(\varepsilon + \varepsilon_F{}^0)\frac{1}{(\omega + i\delta)^2 - \varepsilon^2} \\ &-\lambda\,\mathrm{Im}\int_0^\infty \frac{d\omega}{\pi}\int_{-\omega_D}^{+\omega_D} d\varepsilon\,\mathrm{th}\frac{\omega}{2T_k}\left\{\frac{\nu(\varepsilon + \varepsilon_F{}^0 + \alpha\Delta z\Gamma)}{(\omega + i\Gamma/2)^2 - \varepsilon^2}\right. \\ &\left.\times\frac{\omega + i\Gamma/2}{\omega} - \frac{\nu(\varepsilon + \varepsilon_F{}^0)}{(\omega + i\delta)^2 - \varepsilon^2}\right\}, \qquad \delta \to +0. \end{aligned} \qquad (38)$$

Here the first term determines the T_k for a pure superconductor, neglecting the singularities associated with the topology of the Fermi surface. The second term determines the combined effect on the superconducting transition temperature of singularities in the topology of the Fermi surface and scattering of electrons by impurities. We note that, in the first term in (38), we have omitted the term containing the nonmonotonic correction to the density of states, since we are only interested in the effect of the impurities on the superconducting transition temperature.[2]

We confine our attention to a few limiting cases. If $\varepsilon_F^0 - \varepsilon_k \ll -\omega_D$, then in Eq. (38) the first term plays the major role; for $|\alpha\Delta z\Gamma| \ll \omega_D$ the corrections linear in the impurity concentration are associated with the second term. Therefore, we obtain the following expression for the superconducting transition temperature:

$$T_k = \frac{2\gamma}{\pi}\omega_D\exp\left\{-\frac{1}{\lambda\nu_0(\varepsilon_F{}^0)}\right\}, \qquad (39)$$

where $\ln\gamma = C = 0.577$ is Euler's constant. We note that in this region of Fermi energies ($\varepsilon_F^0 - \varepsilon_k \ll -\omega_D$) the singularity in the density of states does not manifest itself, and the dependence of T_k on the impurity concentration in our examination may only be linear. This is associated with the fact that we neglected the anisotropy of the electron-electron interaction potential.

In the other limiting case, $\varepsilon_F^0 - \varepsilon_k \gg \omega_D$, one also obtains only a linear dependence of T_k on the impurity concentration in the isotropic model of a superconductor. The superconducting transition temperature is determined by formula (39), only $\nu_0(\varepsilon_F)$ must be replaced by the total density of states $\nu(\varepsilon_F)$ on the Fermi surface.

The most interesting behavior of T_k as a function of the concentration occurs for $|\varepsilon_F^0 - \varepsilon_k| \lesssim \omega_D$. We shall consider two cases separately: When the Fermi energy ε_F increases with the addition of impurities (the addition of donor impurities, $\alpha\Delta z\Gamma > 0$), and when the Fermi energy ε_F decreases with the addition of impurities (the addition of acceptor impurities, $\alpha\Delta z\Gamma < 0$).

Let us start with an examination of the case of donor impurities, $\alpha\Delta z\Gamma < 0$. Let $\varepsilon_F^0 = \varepsilon_k$. In order to determine the dependence of T_k on Γ in this case, we explicitly carry out the integration over ε in the second term of Eq. (38). With the use of relation (37), this term is divided into two terms. In the first term containing the smooth function $\nu_0(\varepsilon)$ for the density of states, by virtue of the convergence of the integrand, the limits of the integration over ε may be extended to $\pm\infty$. Applying the theory of residues, we obtain only terms which are linear in Γ (consequently, linear in the impurity concentration as well). If the impurity concentration is such that $\alpha\Delta z \leq \omega_D$, then

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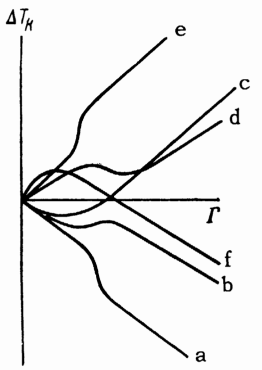
[2] The change of T_k associated with a change of $\epsilon_F{}^0$ under pressure was investigated in[6].



the limits of integration in the second term containing the nonmonotonic correction $\delta\nu$ are $-\alpha\Delta z$ and ω_D. Carrying out the integration over ε and neglecting terms of order T_k/ω_D, we obtain

$$1=\lambda\nu_0(\varepsilon_F{}^0)\ln\frac{2\gamma\omega_D}{\pi T_k}-\lambda A\,\mathrm{Re}\int_0^\infty\frac{d\omega}{2\omega}\mathrm{th}\frac{\omega}{2T_k}\times\left[\left(\alpha\Delta z\Gamma-i\frac{\Gamma}{2}-\omega\right)^{1/2}-(\alpha\Delta z\Gamma-\omega)^{1/2}+\omega^{1/2}-\left(\alpha\Delta z\Gamma+i\frac{\Gamma}{2}+\omega\right)^{1/2}\right].\qquad(40)$$

If $\Gamma/T_k \ll 1$, then from Eq. (40) one can obtain only corrections to T_k which are linear in the concentration. If $\Gamma/T_k \gg 1$, then the increase in the superconducting transition temperature has a nonlinear nature and is described by the formulas

$$\frac{\Delta T_k}{T_k}=\frac{A}{\nu_0}\left[\omega_D{}^{1/2}+\left(\frac{\Gamma}{2}\right)^{1/2}\ln\frac{\Gamma}{T_k}\right]\qquad(41\mathrm{a})$$

for $\alpha\Delta z \ll 1$ and

$$\frac{\Delta T_k}{T_k}=\frac{A}{\nu_0}\left[\omega_D{}^{1/2}+(\alpha\Delta z\Gamma)^{1/2}\ln\frac{\alpha\Delta z\Gamma}{T_k}\right]\qquad(41\mathrm{b})$$

for $\alpha\Delta z \gg 1$.

The first terms in these formulas describe the change of T_k due to the singularity in the density of states $\nu(\varepsilon)$ at $\varepsilon_F^0 = \varepsilon_k$. The second terms describe the change of T_k due to the influence of the impurities. This change, as is evident from formulas (41), is proportional to $n^{1/2}\ln n$, where n is the impurity concentration. Formula (41a) describes the change of T_k when scattering of electrons by impurities plays the major role, and formula (41b)—when the change of the Fermi energy under the influence of, impurities plays the major role. We note that for $A > 0$ we obtain a positive increase of the superconducting transition temperature.

If the Fermi surface of a pure metal does not coincide with the critical isoenergy surface ε_k, then an examination of the transition $\varepsilon_F^0 < \varepsilon_k$ to the critical equal energy surface ε_k is of interest when $\varepsilon_k - \varepsilon_F^0 \gg T_k$.

In the range of concentrations $\Gamma/T_k \ll 1$, the increase of the critical temperature is only linear with respect to the impurity concentration. In connection with the subsequent introduction of impurities in order to achieve concentrations satisfying the condition $\Gamma/T_k \gg 1$, a nonlinear increase of T_k begins even before reaching the critical surface ε_k; this dependence has the same form as in formula (41a).

The effect of the acceptors is described in a similar manner, except that the Fermi energy is decreased by the introduction of acceptors.

The most essential result obtained for the superconducting transition temperature in the cases under consideration is the nonlinear dependence of T_k on the impurity concentration even in a model with an isotropic electron-electron interaction potential. Thus, a change in the topology of the Fermi surface, along with anisotropy of the electron-electron interaction potential, is one of the mechanisms leading to a nonlinear dependence of the superconducting transition temperature on the concentration of impurities. The nonlinear change of T_k with impurity concentration is due to two causes: change of the Fermi energy ε_F and scattering processes. Moreover, the change of T_k caused by the scattering of electrons by impurities depends only on the frequency Γ of electron collisions with impurities, but the change of T_k due to a change of ε_F under the influence of the impurities is different for donor and acceptor impurities. The change of T_k as determined experimentally is the sum of the nonlinear terms and of the linear change of T_k due to the influence of the impurities. Since a linear change of T_k may be both positive as well as negative, and since there are two different possibilities for the nonlinear mechanism (either an increase of T_k, or a decrease of T_k with increase of Γ), there are four possibilities for the total change of T_k with Γ, which are schematically represented in the figure. It should be noted that cases in which there is no initial linear section (curves c and f) may also be observed experimentally.

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