

Effect of dynamic mixing of collectivized and localized states on the critical temperature of superconductors

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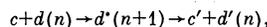
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A model of $d(f)$ metals with localized levels immersed in the conduction band is considered. When the transition energy Ω between the configurations d^{n+1} and d^n is close to the Fermi energy μ , the metal becomes unstable with respect to formation of bound states between the conduction electrons and $d(f)$ ions. As a result, a gap $2\Delta_m$ appears in the conduction band, and the density of states at the edge of the gap is much greater than the initial density. Consequently, Cooper pairing under such conditions may result in superconductivity with a high transition temperature T_c . The conditions on the electron spectrum parameters are obtained and the region of interaction constants λ_m and λ_s , is found for which the gap Δ_m and the superconducting gap Δ , can exist simultaneously.

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1. A characteristic feature of transition d- and rare-earth f-metals and their compounds is the presence in their energy spectra of localized atomic-like levels of $d(f)$ -electrons; for example, the pseudopotential of a transition metal differs from the pseudopotential of an alkali metal by a term which describes the resonance scattering of the conduction electrons by the localized level.^[1] If the localized level (or very narrow band) overlaps the conduction band, then their hybridization (mixing of states) takes place and the density of states in the hybridized bands increases materially close to the level in comparison with the density of states in the trapped conduction band g_0 . We emphasize that the hybridization is due to the action of the crystalline field and is a single-particle effect, which is taken into account in the traditional band scheme.

The scattering of conduction electrons by the level can be regarded as a reaction with a "compound atom" stage:



when the d-ion with a ground n-electron configuration and energy ϵ_n absorbs a conduction electron (c-electron), transforming into an $(n+1)$ electron state with energy ϵ_{n+1} , and then again emits the c-electron, returning to the n electron state. As is shown in^[2,3], if the energy of the transition $\Omega = \epsilon_{n+1} - \epsilon_n$ is sufficiently close to the Fermi energy μ , additional hybridization of the c- and d-states takes place, due to their intra-atomic interaction; in contrast to the usual hybridization (direct mixing), this is known as dynamic mixing. The metallic state for $\mu \sim \Omega$ turns out to be unstable relative to the formation of bound states of the conduction electron with the d-ion, and at a temperature $T = T_m$ it undergoes a phase transition into the "supermixed" state,^[2] which is characterized by the order parameter $\langle c_f^\dagger X_f \sigma^z \rangle$, where c_f^\dagger is the creation operator of the conduction electron at the node f of the crystal lattice, and $X_f \sigma^z$ is the Hubbard operator, which describes the transition of the d-ion from the $(n+1)$ electron configuration to the n electron configuration.

For $T < T_m$, the dispersion law of the quasiparticles in the nonmagnetic case is^[2]

$$E_{\pm}(k) = \frac{1}{2} [\epsilon_k + \Omega \pm \sqrt{(\epsilon_k - \Omega)^2 + 4\tilde{A}^2}] - \mu, \quad (1)$$

where ϵ_k is the energy of the conduction electron and \tilde{A} is the self-consistent parameter of dynamic mixing:

$$\tilde{A} = A(1 - n_0/2), \quad A = -V_m \langle c_r^\dagger X_r \sigma^z \rangle. \quad (2)$$

Here V_m is the potential of the screened intra-atomic Coulomb interaction of c- and d-electrons, n_0 is the relative number of nodes occupied by ions with the n-electron configuration and the mean $\langle c^\dagger X \rangle$ does not depend on the number of nodes. Since the dynamic mixing has a resonance character in the range $\mu \sim \Omega$, the contribution of the crystalline field to the quantity \tilde{A} (single-particle hybridizations) can be neglected. The spectrum (1) determines two subbands: $E_+(k)$ and $E_-(k)$, separated by a forbidden band with a minimum (indirect forbidden band) $E_g \approx 2\Delta_m = 2\tilde{A}^2/W$, which is much less than the value of $2\tilde{A}$ —the direct forbidden band (W is the halfwidth of the conduction band).

Depending on the location of the Fermi level, the supermixed state will either be a dielectric or a state of the type "reduced metal"^[4] with a reduced number of carriers. In both cases, the density of states increases at the edge of the gap (in the integral $\sim 2\tilde{A}$), and, as is shown in^[3],

$$g(E) \sim g_0 \ln \frac{\mu}{|\Omega - \mu|}.$$

The state of the system with $\Delta_m \ll \tilde{A}$ can turn out to be unstable relative to the Cooper pairing, and the energy of coupling of the Cooper band can be much greater than in the initial metal, because of the high density of states.

A similar situation was considered in^[5,6], where the electron-hole pairing leads to a transition metal-dielectric with twice the period of the lattice and formation of a dielectric gap. Similar to our case, the density of states on the edges of the gap increases, which leads to an increase in the binding energy of the Cooper pair and elevation of the temperature of the superconducting transition T_S .

The effect of ordinary hybridization—direct mixing—on the superconductivity was studied in^[7,8], where it was shown that, depending on the relation of the constants of hybridization, intra-atomic interaction and interband interaction, the presence of an unfilled level

near the Fermi surface can lead both to an increase and to a decrease in the effective binding constant and, consequently, in T_S .

In the present paper, we study the superconductivity in the simplest mixing model,^[2] in which the c-electrons fill a simple, nondegenerate s-band, and localized states of the d(f)-ions appear: $|\sigma\rangle$ - n electron configuration with spin $S = 1/2$, its projection σ and energy ϵ_n , $|2\rangle$ - (n + 1) electron configuration with spin $S = 0$ and energy ϵ_{n+1} . The level ϵ_n is assumed to be degenerate in σ (for the magnetic case $\epsilon_{n\uparrow} \neq \epsilon_{n\downarrow}$, the dynamic mixing was considered in^[3]). We shall assume the conduction band to be filled arbitrarily, so that the chemical potential μ can take on different values. The condition of the closeness of Ω and μ is

$$|\Omega - \mu| \leq \mu \exp\{-1/V_m g_0\}.$$

Depending on the quantity $\lambda_m = V_m g_0$, this difference can vary from 10 to 10^3 °K,^[2] so that this limitation on μ is not very severe.

2. We consider the set of collectivized and localized electrons, described by the Hamiltonian

$$\begin{aligned} \mathcal{H} &= \mathcal{H}_0 + \mathcal{H}_{mix} + \mathcal{H}_s, \\ \mathcal{H}_0 &= \sum_{\mathbf{k}\sigma} \xi_{\mathbf{k}} c_{\mathbf{k}\sigma}^+ c_{\mathbf{k}\sigma} + \omega \sum_{\mathbf{r}} X_{\mathbf{r}}^{22}, \\ \mathcal{H}_{mix} &= \sum_{\mathbf{k}\sigma} [A_{\mathbf{r}}(\mathbf{k}) \eta(\sigma) c_{\mathbf{k}\sigma}^+ X_{\mathbf{r}}^{-\sigma,2} + A_{\mathbf{r}}(\mathbf{k}) \eta(\sigma) X_{\mathbf{r}}^{2,-\sigma} c_{\mathbf{k}\sigma}], \\ \mathcal{H}_s &= \sum_{\mathbf{k}_1 \mathbf{k}_2} V_{\mathbf{k}_1 \mathbf{k}_2} c_{\mathbf{k}_1}^+ c_{\mathbf{k}_2}^+ c_{-\mathbf{k}_1} c_{-\mathbf{k}_2}. \end{aligned} \quad (3)$$

Here $c_{\mathbf{k}\sigma}^+$, $c_{\mathbf{k}\sigma}$ are the creation and annihilation operators of the c-electrons with quasimomentum \mathbf{k} and spin σ , $X_{\mathbf{r}}^{pq} \equiv |p\rangle \langle q|$ are the Hubbard operators ($p, q = \sigma, 2$), $\xi_{\mathbf{k}} = \epsilon_{\mathbf{k}} - \mu$, $\omega = \Omega - \mu$, $\eta(\sigma) = \pm 1$ for $\sigma = \pm 1/2$. The Hamiltonian \mathcal{H}_0 describes the set of noninteracting collectivized and localized electrons, \mathcal{H}_{mix} their dynamic mixing with the self-consistent potential $A_{\mathbf{r}}(\mathbf{k})$

$= N^{-1/2} e^{-i\mathbf{k} \cdot \mathbf{r}}$ and \mathcal{H}_s describes the interaction between the c-electrons leading to the superconductivity, while $V_{\mathbf{k}_1 \mathbf{k}_2}$ is the ordinary potential of the BCS attraction model, and is equal to $-V_S$ in the layer $2\omega D$ around the Fermi surface.

We introduce the following anticommutator equal-time Green's function:

$$\begin{aligned} \langle \langle c_{\mathbf{p}\uparrow} | c_{\mathbf{p}\uparrow}^+ \rangle \rangle, \langle \langle X_{\mathbf{r}}^{12} | c_{\mathbf{p}\uparrow}^+ \rangle \rangle, \langle \langle c_{-\mathbf{p}\downarrow}^+ | c_{\mathbf{p}\uparrow}^+ \rangle \rangle, \\ \langle \langle X_{\mathbf{r}}^{21} | c_{\mathbf{p}\uparrow}^+ \rangle \rangle, \end{aligned}$$

the set of equations for the Fourier transforms of which is obtained in the following fashion:^[9]

$$\begin{aligned} (E - \xi_{\mathbf{p}}) \langle \langle c_{\mathbf{p}\uparrow} | c_{\mathbf{p}\uparrow}^+ \rangle \rangle_{\mathbf{E}} - \sum_{\mathbf{r}} A_{\mathbf{r}}(\mathbf{p}) \langle \langle X_{\mathbf{r}}^{12} | c_{\mathbf{p}\uparrow}^+ \rangle \rangle_{\mathbf{E}} + \Delta(\mathbf{p}) \langle \langle c_{-\mathbf{p}\downarrow}^+ | c_{\mathbf{p}\uparrow}^+ \rangle \rangle_{\mathbf{E}} &= 1, \\ (E - \omega) \langle \langle X_{\mathbf{r}}^{12} | c_{\mathbf{p}\uparrow}^+ \rangle \rangle_{\mathbf{E}} - (1 - n_+) \sum_{\mathbf{k}} A_{\mathbf{r}}(\mathbf{k}) \langle \langle c_{\mathbf{k}\uparrow} | c_{\mathbf{p}\uparrow}^+ \rangle \rangle_{\mathbf{E}} &= 0, \\ (E + \xi_{\mathbf{p}}) \langle \langle c_{-\mathbf{p}\downarrow}^+ | c_{\mathbf{p}\uparrow}^+ \rangle \rangle_{\mathbf{E}} - \sum_{\mathbf{r}} A_{\mathbf{r}}(-\mathbf{p}) \langle \langle X_{\mathbf{r}}^{21} | c_{\mathbf{p}\uparrow}^+ \rangle \rangle_{\mathbf{E}} + \Delta^*(\mathbf{p}) \langle \langle c_{\mathbf{p}\uparrow} | c_{\mathbf{p}\uparrow}^+ \rangle \rangle_{\mathbf{E}} &= 0, \\ (E + \omega) \langle \langle X_{\mathbf{r}}^{21} | c_{\mathbf{p}\uparrow}^+ \rangle \rangle_{\mathbf{E}} - (1 - n_-) \sum_{\mathbf{k}} A_{\mathbf{r}}(-\mathbf{k}) \langle \langle c_{-\mathbf{k}\downarrow} | c_{\mathbf{p}\uparrow}^+ \rangle \rangle_{\mathbf{E}} &= 0. \end{aligned} \quad (4)$$

Here

$$\Delta(\mathbf{p}) = - \sum_{\mathbf{k}} V_{\mathbf{p}\mathbf{k}} \langle \langle c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} \rangle \rangle, \quad n_{\sigma} = \langle X_{\mathbf{r}}^{\sigma\sigma} \rangle, \quad \langle \dots \rangle = \frac{\text{Sp}(\dots e^{-\mathcal{H}/T})}{\text{Sp} e^{-\mathcal{H}/T}}. \quad (5)$$

In the nonmagnetic case $n_+ = n_- = 1/2 n_0$. Assuming $\Delta(\mathbf{p})$ to be a real quantity, we find the solution of (4):

$$\begin{aligned} \langle \langle c_{\mathbf{p}\uparrow} | c_{\mathbf{p}\uparrow}^+ \rangle \rangle_{\mathbf{E}} &= \frac{E + \xi_{\mathbf{p}} - \bar{A}^2 / (E + \omega)}{D_{\mathbf{p}}(E)}, \quad \langle \langle c_{-\mathbf{p}\downarrow}^+ | c_{\mathbf{p}\uparrow}^+ \rangle \rangle_{\mathbf{E}} = - \frac{\Delta(\mathbf{p})}{D_{\mathbf{p}}(E)}, \\ \langle \langle X_{\mathbf{r}}^{12} | c_{\mathbf{p}\uparrow}^+ \rangle \rangle_{\mathbf{E}} &= \frac{A_{\mathbf{r}}(\mathbf{p}) (1 - n_0 / 2) E + \xi_{\mathbf{p}} - \bar{A}^2 / (E + \omega)}{E - \omega} \frac{E + \xi_{\mathbf{p}} - \bar{A}^2 / (E + \omega)}{D_{\mathbf{p}}(E)}, \\ \langle \langle X_{\mathbf{r}}^{21} | c_{\mathbf{p}\uparrow}^+ \rangle \rangle_{\mathbf{E}} &= \frac{-A_{\mathbf{r}}(-\mathbf{p}) (1 - n_0 / 2) \Delta(\mathbf{p})}{E + \omega} \frac{\Delta(\mathbf{p})}{D_{\mathbf{p}}(E)} \end{aligned} \quad (6)$$

where

$$D_{\mathbf{p}}(E) = \frac{1}{E^2 - \omega^2} \{ [(E - \xi_{\mathbf{p}})(E - \omega) - \bar{A}^2] [(E + \xi_{\mathbf{p}})(E + \omega) - \bar{A}^2] - \Delta^2(\mathbf{p})(E^2 - \omega^2) \}. \quad (7)$$

The functions (6) still do not give complete information on the system; for calculation of averages of the type $\langle X^{\sigma\sigma} \rangle$ and $\langle X^{22} \rangle$, we must know the functions

$$\langle \langle X_{\mathbf{r}}^{\sigma 2} | X_{\mathbf{r}}^{2\sigma} \rangle \rangle, \quad \langle \langle c_{\mathbf{k}\sigma} | X_{\mathbf{r}}^{2\sigma} \rangle \rangle, \quad \langle \langle c_{-\mathbf{k}\sigma}^+ | X_{\mathbf{r}}^{2\sigma} \rangle \rangle, \quad \langle \langle X_{\mathbf{r}}^{2,-\sigma} | X_{\mathbf{r}}^{2\sigma} \rangle \rangle,$$

which are easily found from the set of equations similar to the set (4):

$$\begin{aligned} \langle \langle X_{\mathbf{r}}^{12} | X_{\mathbf{r}}^{21} \rangle \rangle_{\mathbf{E}} &= \frac{1 - n_0 / 2}{E - \omega} + \sum_{\mathbf{p}} \frac{\bar{A}^2 (1 - n_0 / 2) E + \xi_{\mathbf{p}} - \bar{A}^2 / (E + \omega)}{(E - \omega)^2} \frac{E + \xi_{\mathbf{p}} - \bar{A}^2 / (E + \omega)}{D_{\mathbf{p}}(E)}, \\ \langle \langle c_{\mathbf{p}\uparrow} | X_{\mathbf{r}}^{21} \rangle \rangle_{\mathbf{E}} &= \frac{A_{\mathbf{r}}(\mathbf{p}) (1 - n_0 / 2) E + \xi_{\mathbf{p}} - \bar{A}^2 / (E + \omega)}{E - \omega} \frac{E + \xi_{\mathbf{p}} - \bar{A}^2 / (E + \omega)}{D_{\mathbf{p}}(E)}, \\ \langle \langle c_{-\mathbf{p}\downarrow}^+ | X_{\mathbf{r}}^{21} \rangle \rangle_{\mathbf{E}} &= \frac{-A_{\mathbf{r}}(\mathbf{p}) (1 - n_0 / 2) \Delta(\mathbf{p})}{E - \omega} \frac{\Delta(\mathbf{p})}{D_{\mathbf{p}}(E)}, \\ \langle \langle X_{\mathbf{r}}^{21} | X_{\mathbf{r}}^{21} \rangle \rangle_{\mathbf{E}} &= - \sum_{\mathbf{p}} \frac{\bar{A}^2 (1 - n_0 / 2) \Delta(\mathbf{p})}{E^2 - \omega^2} \frac{\Delta(\mathbf{p})}{D_{\mathbf{p}}(E)}. \end{aligned} \quad (8)$$

The expression for $D_{\mathbf{p}}(E)$ is conveniently written in the form

$$D_{\mathbf{p}}(E) = \frac{1}{E^2 - \omega^2} \{ [E^2 - E_{+}^2(\mathbf{p})] [E^2 - E_{-}^2(\mathbf{p})] - \Delta^2(\mathbf{p})(E^2 - \omega^2) \},$$

where $E_{\pm}(\mathbf{p})$ are determined by Eq. (1). The excitation spectrum is determined from the equation $D_{\mathbf{p}}(E) = 0$:

$$E_{1,2}^2(\mathbf{p}) = 1/2 \{ E_{+}^2(\mathbf{p}) + E_{-}^2(\mathbf{p}) + \Delta^2(\mathbf{p}) \pm [(E_{+}^2(\mathbf{p}) - E_{-}^2(\mathbf{p}))^2 + \Delta^2(\mathbf{p})(\Delta^2(\mathbf{p}) + 2(E_{+}^2(\mathbf{p}) + E_{-}^2(\mathbf{p}) - 4\omega^2))]^{1/2} \}. \quad (9)$$

In the limiting case $\Delta(\mathbf{p}) \rightarrow 0$, the spectrum (9) goes over into (1) and, as $A \rightarrow 0$, $\omega \rightarrow 0$, we get the usual form of the dispersion law in a superconductor.

3. We find the averages of interest to us with the help of the spectral theorem:

$$\begin{aligned} \langle \langle c_{\mathbf{p}\uparrow}^+ c_{\mathbf{p}\uparrow} \rangle \rangle &= \frac{1}{2} - \frac{1}{E_1^2(\mathbf{p}) - E_2^2(\mathbf{p})} \left\{ \frac{\xi_{\mathbf{p}}(E_1^2(\mathbf{p}) - \omega^2) + \omega \bar{A}^2}{2E_1(\mathbf{p})} \text{th} \frac{E_1(\mathbf{p})}{2T} \right. \\ &\quad \left. - \frac{\xi_{\mathbf{p}}(E_2^2(\mathbf{p}) - \omega^2) + \omega \bar{A}^2}{2E_2(\mathbf{p})} \text{th} \frac{E_2(\mathbf{p})}{2T} \right\}, \end{aligned} \quad (10)$$

$$\begin{aligned} \langle \langle c_{\mathbf{p}\uparrow}^+ c_{-\mathbf{p}\downarrow}^+ \rangle \rangle &= \frac{\Delta(\mathbf{p})}{E_1^2(\mathbf{p}) - E_2^2(\mathbf{p})} \left\{ \frac{E_1^2(\mathbf{p}) - \omega^2}{2E_1(\mathbf{p})} \text{th} \frac{E_1(\mathbf{p})}{2T} \right. \\ &\quad \left. - \frac{E_2^2(\mathbf{p}) - \omega^2}{2E_2(\mathbf{p})} \text{th} \frac{E_2(\mathbf{p})}{2T} \right\}, \end{aligned} \quad (11)$$

$$\begin{aligned} \langle \langle c_{\mathbf{p}\uparrow}^+ X_{\mathbf{r}}^{12} \rangle \rangle &= \frac{-A_{\mathbf{r}}(\mathbf{p})}{E_1^2(\mathbf{p}) - E_2^2(\mathbf{p})} \left\{ \frac{E_1^2(\mathbf{p}) + \omega \xi_{\mathbf{p}} - \bar{A}^2}{2E_1(\mathbf{p})} \text{th} \frac{E_1(\mathbf{p})}{2T} \right. \\ &\quad \left. - \frac{E_2^2(\mathbf{p}) + \omega \xi_{\mathbf{p}} - \bar{A}^2}{2E_2(\mathbf{p})} \text{th} \frac{E_2(\mathbf{p})}{2T} \right\}. \end{aligned} \quad (12)$$

The expressions for the averages $\langle X_{\mathbf{r}}^{23} \rangle = \langle X_{\mathbf{r}}^{\uparrow 2} X_{\mathbf{r}}^{\downarrow 2} \rangle$ and $\langle X_{\mathbf{r}}^{\sigma\sigma} \rangle = \langle X_{\mathbf{r}}^{\sigma 2} X_{\mathbf{r}}^{2\sigma} \rangle$ are found in a similar way from (8). The explicit values of these averages is not given because of their cumbersome nature.

Using the definitions (2) and (5) and the relations (11) and (12), we find the self-consistent equations for A and the superconducting gap Δ_S (for simplicity, we consider a rectangular conduction band with the level $\mu_0 = 0$ set at the middle of the band):

$$\frac{1}{\lambda_s} = \frac{1}{2} \int_{-\omega_D}^{\omega_D} \frac{d\xi}{E_1^2(\xi) - E_2^2(\xi)} \left\{ \frac{E_1^2(\xi) - \omega^2}{E_1(\xi)} \operatorname{th} \frac{E_1(\xi)}{2T} - \frac{E_2^2(\xi) - \omega^2}{E_2(\xi)} \operatorname{th} \frac{E_2(\xi)}{2T} \right\}, \quad (13)$$

$$\frac{1}{\lambda_m} = \frac{1}{2} \int_{-W}^W \frac{d\xi}{E_1^2(\xi) - E_2^2(\xi)} \left\{ \frac{E_1^2(\xi) + \omega\xi - \bar{A}^2}{E_1(\xi)} \operatorname{th} \frac{E_1(\xi)}{2T} - \frac{E_2^2(\xi) + \omega\xi - \bar{A}^2}{E_2(\xi)} \operatorname{th} \frac{E_2(\xi)}{2T} \right\}. \quad (14)$$

Here $\lambda_S = V_{SG}0$ and $\lambda_M = V_{MG}0$. The equation for the chemical potential has the form

$$n = n_e + n_i + 2n_z = \frac{1}{N} \sum_{k\sigma} \langle c_{k\sigma}^\dagger c_{k\sigma} \rangle + \langle X^{++} \rangle + \langle X^{+-} \rangle + 2\langle X^{zz} \rangle, \quad (15)$$

where n is the given electron concentration. In an alloyed metal, or in an intermetallic compound with a complicated unit cell, the quantity n may not be an integer. Correspondingly, the Fermi level will lie not at the middle of the conduction band: $\mu = \mu_0 - \delta\mu = -\delta\mu$.

Equations (13), (14) and (15) form a system from which the order parameters Δ_S , A and the chemical potential μ can be obtained in principle as a function of the interaction constants λ_S , λ_M and the temperature T . The existence of common solutions with nonzero Δ_S and A would mean a superconducting state of the system with dynamic mixing.

4. We now determine under what conditions, imposed on the parameters λ_N , λ_S , ω , ω_D and $\delta\mu$, does a non-trivial solution for Δ_S appear. In this case, we set $\Delta_S = +0$ in Eqs. (13), (14). For $\delta\mu < 2\Delta_M$ and $\omega = 0$ we find from Eq. (13)

$$\bar{A} = \frac{\omega_D}{2} \exp \left\{ -\frac{1}{\lambda_s} \right\}. \quad (16)$$

Equation (14) takes the form

$$\frac{1}{\lambda_m} \approx \operatorname{arsh} \frac{W}{2\bar{A}} + \frac{\bar{A}^2}{\bar{A}^2 + \omega_D^2} \frac{1}{2} \left\{ \operatorname{arsh} \frac{\bar{A}}{2\Delta_M - \delta\mu} + \operatorname{arsh} \frac{\bar{A}}{2\Delta_M + \delta\mu} \right\}. \quad (17)$$

As $\delta\mu \rightarrow 0$, (17) takes on the solution obtained earlier in^[2]:

$$\bar{A}_0 = \frac{W}{2} \exp \left\{ -\frac{1}{2\lambda_m} \right\}. \quad (18)$$

Comparing (16) and (18), we see that in the limit $\delta\mu \rightarrow 0$, the condition

$$\operatorname{sh} \frac{1}{\lambda_s} = \frac{\omega_D}{W} \operatorname{sh} \frac{1}{2\lambda_m}, \quad (19)$$

is necessary for the compatibility of the system; for finite λ_M , this relation is satisfied only for finite λ_S i.e., there is a threshold in the interaction constant. The condition (19) means the necessity of a strong attraction for the formation of Cooper pairs, when the chemical potential lies within the gap $2\Delta_M$. The condition (19) can be satisfied also for $\lambda_M \rightarrow 0$ and $\lambda_S \rightarrow 0$, which means the identity of the temperatures T_M and T_S . We shall not consider this case.

In the other limit $2\Delta_M - \delta\mu \ll 2\Delta_M$, Eq. (17) has the form

$$\frac{1}{\lambda_m} = \operatorname{arsh} \frac{W}{2\bar{A}} + \frac{1}{2} \operatorname{arsh} \frac{\bar{A}}{2\Delta_M - \delta\mu}. \quad (20)$$

Substituting (16) in (20) we find the desired condition on the parameters

$$\frac{1}{\lambda_m} = \operatorname{arsh} \frac{W}{2\bar{A}} + \frac{1}{2} \operatorname{arsh} \left(\frac{\omega_D \exp\{-1/\lambda_s\}}{2\Delta_M - \delta\mu} \right), \quad (21)$$

which is satisfied for finite λ_M for as weak an attraction as is suitable. The condition (21) illustrates the fact that as $\delta\mu \rightarrow 2\Delta_M$, the Fermi level falls into the energy range with a high density of states. It is natural to expect that the temperature of the superconducting transition T_S will in this case be much greater than the temperature T_{S0} —the critical temperature of the superconductor in the absence of mixing.

5. To obtain T_S , we set $\Delta_S = +0$ in Eqs. (13), (14):

$$\begin{aligned} \frac{1}{\lambda_s} = & \int_{-\omega_D}^{\omega_D} \frac{d\xi}{(\xi + \delta\mu)(\xi^2 + 4\bar{A}^2)^{1/2}} \frac{1}{4} \left\{ [\xi + \delta\mu + \sqrt{\xi^2 + 4\bar{A}^2}] \right. \\ & \times \operatorname{th} \frac{\sqrt{\xi^2 + 4\bar{A}^2} + \xi + \delta\mu}{4T} + [\xi + \delta\mu - \sqrt{\xi^2 + 4\bar{A}^2}] \operatorname{th} \frac{\sqrt{\xi^2 + 4\bar{A}^2} - \xi - \delta\mu}{4T} \left. \right\}, \\ \frac{1}{\lambda_m} = & \int_{-W}^W \frac{d\xi}{(\xi + \delta\mu)(\xi^2 + 4\bar{A}^2)^{1/2}} \frac{1}{4} \left\{ \frac{E_+^2(\xi) - \bar{A}^2}{E_+(\xi)} \operatorname{th} \frac{\sqrt{\xi^2 + 4\bar{A}^2} + \xi + \delta\mu}{4T} \right. \\ & \left. + \frac{E_-^2(\xi) - \bar{A}^2}{E_-(\xi)} \operatorname{th} \frac{\sqrt{\xi^2 + 4\bar{A}^2} - \xi - \delta\mu}{4T} \right\} \end{aligned} \quad (22)$$

Equations (22) are written for the case $\omega = 0$ under the assumption that $T_M > T_S$; then Δ_M differs from zero for $T = T_S$. Moreover, we shall assume that the chemical potential $\mu = -\delta\mu$ is the specified parameter and not the concrete specification of the electrons n .

The set of Eqs. (22) was solved by means of a high-speed computer. As the calculations show, there exists a three-dimensional region G in the space of the parameters λ_0 , λ_M , $\delta\mu$ inside which the system is compatible. For the intersections of G with the planes $\delta\mu = \text{const}$, the character of the phase transition on the boundary curve will be different for different $\delta\mu$: for $\delta\mu = 0$, it is a first order transition (see (19)), for $\delta\mu = 2\Delta_M$, a second order (see (20)), and for $\delta\mu < 2\Delta_M$, first order close to a second order transition (intermediate case). Figure 1 shows the section of the region G with $\delta\mu < 2\Delta_M$ for which T_S/T_{S0} reaches a maximum (see Fig. 2); here a maximum of T_S/T_{S0} on the plane λ_S , λ_M is achieved on the line AL (T_{S0} is determined from (22) for $\bar{A} = 0$ and coincides with the BCS formula only for $\delta\mu = 0$). It should be noted that for $\delta\mu = 0$, the existence of compatible solutions is accidental in this sense that there is only one line (see (19)) on the plane λ_S , λ_M while for $\delta\mu \neq 0$, there is an entire region.

Some of the solutions of the system for different λ_S , λ_M , and $\delta\mu$ are given in the table, from which it is seen that the maximal ratio T_S/T_{S0} is greater than 40 and the maximal T_S is equal to 30°K. The considered region of values of the constants λ_S and λ_M is entirely real, since, for example, for superconductors, λ_S lies in the interval 0.18 (Zn, Al) to 0.39 (Pb),^[10] while the mixing constant λ_M , according to^[2], is in the range 0.1 $\lambda_M < 0.2$.

All the obtained solutions of T_S/T_{S0} have sharp maxima in the parameter $(2\Delta_M - \delta\mu)/2\Delta_{M0}$ for $2\Delta_M - \delta\mu < 0$ (Fig. 2). This result shows that the maximum amplification of T_S/T_{S0} takes place when the Fermi level lies in the range of forbidden values of energy with an increased density of states. Upon further increase of $\delta\mu$, the Fermi level gets into a region far from ω , where the mixing no longer adds to the density of states.

The condition of applicability of Eqs. (22) $T_S < T_M$

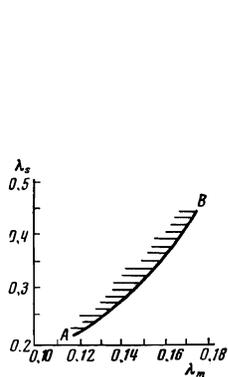


FIG. 1

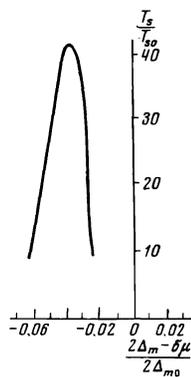


FIG. 2

FIG. 1. Region of points (λ_s, λ_m) (shaded) allowing compatible solution of the set of equations (22) for $\omega_D/W = 0.03$.

FIG. 2. Dependence of T_s/T_{s0} on $(2\Delta_m - \delta\mu)/2\Delta_{m0}$ for $\lambda_s = 0.331$, $\lambda_m = 0.153$ and $\omega_D/W = 0.03$.

Some solutions of the set of equations (22) for the points (λ_s, λ_m) lying on the curve AB

λ_s	λ_m	$\delta\mu, K$	T_{s0}, K	T_s, K	$\bar{\lambda}, K$	T_s/T_{s0}
0.204	0.116	0.2	0.08	2	0.44	25
0.232	0.122	4.1	1.2	3	2.3	2.5
0.257	0.132	0.9	1.5	5.7	3.5	3.8
0.264	0.134	0.2	0.21	6.5	4	30.9
0.331	0.153	0.15	0.4	16.5	2.6	41.2
0.331	0.153	0.2	0.7	16.5	2.6	23.6
0.398	0.166	10	4	24	10	6
0.403	0.168	13.5	12	22	6	1.8
0.438	0.173	13.9	6	30	8	5
0.444	0.173	13.5	4	30	15	7.5

is satisfied for all the solutions obtained: thus, if we "come down" from the high temperature region, then a succession of transitions takes place: metal—"reduced metal"—superconductor.

6. We have assumed the level to be infinitesimally narrow; if it diffuses into a narrow band of width Γ , then, so long as $\Gamma < 2\Delta_m$, nothing changes qualitatively; only the indirect forbidden band narrows (in the case of identical signs of the effective masses of the broad and narrow bands in the region of their overlap). Even for $\Gamma > 2\Delta_m$ the basic conclusion on the increase in T_s/T_{s0} remains in force, since the peak in the density of states remains, although the indirect forbidden band vanishes.

We also note that the increase in T_s/T_{s0} will take place in the case in which the mixing will not be dynamic (many-particle), but the usual single-particle hybridization.^[7]

The considered model applies to compounds of transition or rare-earth metals, in which the localized level lies near the Fermi level. The necessary closeness can be achieved by alloying. Evidently such a situation

exists in the layered compounds Me_xMoS_2 ,^[11] where Me is an alkali metal. For $x = 0.3-0.4$, the value of T_s increases to 6.3°K from 1.7°K in pure MoS_2 .

In addition, our model can possibly be applicable to intermetallic components with a complicated unit cell, for example, with the structure $\beta - W$, about which it is known that near the Fermi level, at a distance ~ 0.01 eV, a narrow peak is found in the density of states.^[12] This peak is usually explained by the quasi-one-dimensional motion of the electrons connected with the specific symmetry of the structure $\beta - W$; Account of the band structure of these compounds,^[13] carried out with account of the lattice symmetry and with account of single-particle hybridization, confirms the presence of a peak in the density of states, but the value of the density of states in^[13] was obtained almost an order of magnitude less than the experimental value. Possibly the dynamic mixing considered above also leads to such a large density of states.

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