Description of the Coulomb interaction in the theory of superconductivity and calculation of T_c

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A method is proposed for solving the Éliashberg equation for anisotropic superconductors in the temperature technique at $T = T_c$. The solution is found by successive calculation of the terms of order $\lambda\ln(\omega_D/T_c)$, λ, λ^2,..., where $\lambda = \lambda_0/(1+\lambda_0)$ is the renormalized electron-phonon coupling constant. A consistent way of taking the Coulomb interaction of the electrons into account is described and a definition of the Coulomb pseudopotential in the anisotropic model is given. A general expression for T_c, including corrections of order λ, is given. The dependence of the effective mass on the energy gives a contribution to the corrections of order λ^2 and higher. For the Einstein model T_c is calculated to order λ^2. For a model in which the phonon spectrum consists of two Einstein peaks the equations are solved numerically and the dependence of T_c of the frequency ω_1 of one of the peaks is determined. It is shown that as $\omega_1 \to 0$ this peak gives a finite contribution to T_c if $\lambda_1 \sim \omega_1^{-2}$. If $\lambda_1 \sim \omega_1^{-2+\nu}$, where $\nu > 0$, the contribution from the low-frequency peak vanishes in the limit $\omega_1 \to 0$.

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There are a large number of papers devoted to deriving an approximate analytic formula for the T_c of strong-coupling superconductors. (Such attempts are undertaken with the purpose of going beyond the framework of the BCS approximation, in order to describe the experimental situation.) The best-known is the empirical formula of McMillan[1]:

$$T_c = \frac{\Theta}{1.45}\exp\left[-\frac{1.04(1+\lambda_0)}{\lambda_0-\mu^*(1+0.62\lambda_0)}\right], \qquad (1)$$

which was obtained by fitting the results of a numerical solution of the Éliashberg equation to a simple analytic form[2]. An electron-phonon interaction function $\alpha^2(\omega)F(\omega)$ extracted from tunneling measurements on niobium was used. Here,

$$\lambda_0 = 2\int_0^\infty \alpha^2(\omega)F(\omega)\,d\omega/\omega$$

is the electron-phonon coupling constant, μ^* is the Coulomb pseudo-potential and Θ is the Debye temperature. Although formula (1) is valid just for niobium, it is often applied to any superconducting metal, even though in such cases there are no adequate reasons for preferring the McMillan formula to the BCS formula. The attempts to obtain an empirical formula of the same type for other superconductors are well-known[3-7]. These formulas differ from (1) in the numerical coefficients, and all of them are nonuniversal, since they pertain to superconductors with specific phonon spectrum. In recent papers[8-11], expressions of a more general type for T_c are derived. In these formulas, functionals of $\alpha^2(\omega)F(\omega)$ appear in the role of the numerical coefficients. To derive these formulas[10,11] one uses approximate solutions of the Éliashberg equation, obtained, e.g., by substituting a step function or the Morel-Anderson function[12] as a first approximation for the gap function $\Delta(\omega)$. No attempts are made to estimate the accuracy of the approximation, inasmuch as the procedure turns out to be extremely cumbersome even in the first stage. In essence, such a procedure corresponds to determining the first correction in the constant $\lambda = \lambda_0/(1+\lambda_0)$ to the exponential factor $\lambda - \mu^*$ and is valid for sufficiently small λ_0. In particular, it cannot be used to elucidate the question of the influence of the low-frequency phonon peaks on the magnitude of T_c if the coupling constant for the coupling with the low-frequency mode is large. The erroneous result obtained in[10,11] concerning the role of the soft phonon modes is connected with this fact.

It should be noted that the solution of the Éliashberg equation, like the form of the equation itself, is considerably simplified in the temperature technique[13], since in this representation all quantities are real and the kernel has no singularities. Formulas for T_c going beyond the framework of the first approximation were obtained in the temperature technique in[14] for phonon spectra with one and two Einstein modes.

In this paper we shall describe a regular method for solving the Éliashberg equation in the temperature technique for the general case of an anisotropic superconductor with an arbitrary phonon spectrum. The solution is represented in the form of a series in powers of the electron-phonon interaction. We shall derive a strong-coupling formula for T_c in the anisotropic model and shall calculate T_c in certain particular cases; we shall also consider the question of the effect on T_c of the low-frequency phonon peaks.

1. DERIVATION OF THE EQUATIONS

The Coulomb interaction of the electrons in a superconductor has been taken into account most consistently by Batyev[15] in the framework of the isotropic model. We shall formulate the corresponding result, having modified it for a variant of the temperature technique, without assuming that the interaction is isotropic. The equation for the determination of T_c has the form

$$\Delta_{np} = -T\sum_m \int \frac{dp'}{(2\pi)^3}(D_{pp'}^{nm}+K_{pp'}^{nm})R_{mp'}\Delta_{mp'}, \qquad (2)$$

where

$$D_{pp'}^{nm} = -\sum_j |g_{pp'}^j|^2 \frac{\omega_{j,\,p-p'}^2}{\omega_{j,\,p-p'}^2 + \omega_{n-m}^2}; \qquad (3)$$

$g_{pp'}^j$ is the total (with allowance for all the Coulomb corrections) amplitude for scattering of an electron by a phonon with the j-th polarization; $K_{pp'}^{nm}$ is the total Coulomb amplitude; $R_{np} = G_{np}G_{-n,-p}$ where G_{np} is the normal electron Green function, which near the Fermi surface has the form

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$$G_{np}=\frac{a_s}{i\omega_n-f_{ns}-\varepsilon_p}. \quad (4)$$

The residue a_s (at the point s on the Fermi surface) and the electron spectrum ϵ_p are determined without allowance for the electron-phonon interaction. The function f_{ns} is defined by the expression

$$f_{ns}=i\pi TN(0)\sum_m\int d\tau_{s'}a_sD_{ss'}^{nm}a_{s'}\operatorname{sgn} m;$$

$$d\tau_s=\frac{ds}{(2\pi)^3v_sN(0)}. \quad (5)$$

where v_s is the velocity and $N^{(0)}$ is the density of states at the Fermi surface, without allowance for the electron-phonon interaction. It is well-known that formulas (2)—(5) are valid to within terms $\sim\lambda\omega_D/\epsilon_F$.

Owing to the existence of two characteristic interaction dimensions (ω_D for the electron-phonon interaction and ϵ_F for the Coulomb interaction), it turns out to be possible[15] to represent the function Δ_{np} in the form of a sum

$$\Delta_{np}=\Phi_{ns}-\chi_{np} \quad (6)$$

of a rapidly varying contribution Φ_{ns}, concentrated in the region of frequencies $|\omega_n|\lesssim\omega_D$, and a smooth contribution χ_{np} with a characteristic region of variation $\sim\epsilon_F$. The dependence on p is smooth for both contributions. From the definition of the functions Φ and χ, Eq. (2) breaks down into two equations, which we shall write in the symbolic form

$$\Phi=DR(\Phi-\chi);\quad \chi=KR(\Phi-\chi). \quad (7)$$

After integrating over the energy, we obtain for the function Φ_{ns} an equation in which the smooth part is represented by its boundary value (in both variables) χ_{0s} on the Fermi surface:

$$\Phi_{ns}=-\pi TN(0)\sum_m\int d\tau_{s'}D_{ss'}^{nm}a_{s'}^2\frac{\Phi_{ms'}-\chi_{0s'}}{|\omega_m+f_{ms'}|}. \quad (8)$$

In the equation for χ_{np} the term $KR\Phi$ contains, under the integral, the rapidly varying function Φ, which brings the integral out on to the Fermi surface. We shall represent the function R in the form $R = R^C + \Delta R$, separating out the contribution from the electron-phonon interaction. This contribution, like Φ, is concentrated near the Fermi surface. Now the equation for χ takes the form

$$(1+KR^c)\chi=K(R\Phi-\chi\Delta R).$$

The left-hand side of this equation contains a term that depends logarithmically on the temperature. This term arises from the summation in the region of low frequencies. Indeed, for $|\omega_m|\ll\epsilon_F$,

$$\int R_c(p'\omega_m)d\varepsilon_{p'}=\frac{\pi a_{s'}^2}{|\omega_m|}$$

and subsequent summation over the frequencies gives the logarithm. With the aim of determining the Coulomb-pseudo-potential with the aid of the equation for χ, we shall separate out the contribution from the low frequencies in explicit form. For this we shall introduce the function $\eta_{\omega_m}^{\omega_0}=\omega_m^2/(\omega_0^2+\omega_m^2)$, which cuts off the lower limit of the sum over $|\omega_m|$, and write

$$(1+KR_c\eta^{\omega_0})\chi=K(R\Phi-R\bar\eta^{\omega_0}\chi-\eta^{\omega_0}\chi\Delta R), \quad (9)$$

where $\bar\eta_{\omega_m}^{\omega_0}=1-\eta_{\omega_m}^{\omega_0}=\omega_0^2/(\omega_0^2+\omega_m^2)$. The frequency $\omega_0\sim\omega_D$ will be defined below. In the right-hand side of Eq. (9) the sum over the frequencies ω_m and the integral over the energy ϵ' converge in the region ϵ', $|\omega_m|\lesssim\omega_D$. Therefore, the amplitude $K_{pp'}^{nm}$ in the right-hand side of the equation can be put equal to $K_{ps'}^{n0}$, and the boundary value $\chi_{0s'}$ substituted for the smooth function $\chi_{np'}$. We shall write the right-hand side in the form

$$\int d\tau_{s'}N(0)K_{ps'}^{n0}a_{s'}{}^2b_{s'},$$

where

$$b_{s'}=\pi T\sum_m\left[\frac{\Phi_{ms'}-\bar\eta_m^{\omega_0}\chi_{0s'}}{|\omega_m+if_{ms'}|}+\left(\frac{1}{|\omega_m|}-\frac{1}{|\omega_m+if_{ms'}|}\right)\eta_m^{\omega_0}\chi_{0s'}\right]. \quad (10)$$

The function $a_s^2{}'b_{s'}$ can be eliminated from Eq. (9) if we seek the solution in the form

$$\chi_{np}=\int\psi_{ps'}^n a_{s'}^2b_{s'}d\tau_{s'}. \quad (11)$$

We note that in the left-hand side of Eq. (9) it is possible, making an error of order $(\pi T/\omega_0)^2$, to change from the discrete variables ω_n and ω_m to continuous variables x and y and replace the sum by an integral. Using this fact and substituting (11) into (9), we obtain an equation for $\psi_{ps'}^x$:

$$\psi_{ps'}^x+\frac{1}{\pi}\int_0^\infty dy\int\frac{dp_1}{(2\pi)^3}K_{pp_1}^{xy}R_{yp_1}^c\eta_y^{\omega_0}\psi_{p_1s'}^y=N(0)K_{ps'}^{x0}, \quad (12)$$

which does not depend on the temperature and contains the variable s' as a parameter. Eq. (12) has a single solution. Introducing for the boundary value $\psi_{ss'}^0$ the notation

$$\mu_{ss'}^*=a_s\psi_{ss'}^0a_{s'}, \quad (13)$$

we obtain the following equation for χ_{0s}:

$$a_s\chi_{0s}=\int d\tau_{s'}\mu_{ss'}^*a_{s'}b_{s'}. \quad (14)$$

The relation (13) together with Eq. (12) determines the Coulomb pseudo-potential $\mu_{ss'}^*$. The matrix $\mu_{ss'}^*$ is symmetric, since the kernel $K_{pp'}^{xy}$ is symmetric. We shall not concern ourselves with solving Eq. (12), since this has only a formal meaning, inasmuch as it is impossible, generally speaking, to calculate the Coulomb kernel K. We note, however, that Eq. (12) has a small parameter $\ln^{-1}(\epsilon_F/\omega_0)$, which arises owing to the logarithmic contribution of the low frequencies to the integral in the left-hand side. In the leading approximation in $\ln^{-1}(\epsilon_F/\omega_0)$ it is necessary to take ψ on the Fermi surface. For example, in the isotropic model in this approximation,

$$\mu^*=a^2N(0)\overline{K_{ss'}^{00}}\left(1+\frac{1}{\pi}\int_0^\infty dy\int\frac{dp_1}{(2\pi)^3}\overline{K_{sp_1}^{0y}}R_{yp_1}^c\eta_y^{\omega_0}\right)^{-1}. \quad (15)$$

The bar denotes averaging over the Fermi surface. For a system of high density, when the random-phase approximation is valid, we obtain from (15) the well-known result[12]

$$\mu^*=\frac{\mu_0}{1+\mu_0\ln(4\varepsilon_F/\omega_0)};\qquad \mu_0=\frac{1}{2\pi v}\ln\pi v.$$

Here v is the Fermi velocity in atomic units and $1/\pi v$ is the small parameter of the high-density model.

In order to bring Eqs. (8) and (14) to a form convenient for analysis, we introduce the notation

$$\Lambda_{ss'}^0(\omega)=N(0)\sum_j a_s|g_{ss'}^j|^2a_{s'}\delta(\omega_{jss'}^2-\omega^2) \quad (16)$$

and represent the function if_{ns} in the form

$$if_{ns}=\pi T\sum_m\int_0^\infty d\omega^2\int d\tau_{s'}\,\overline{\eta}^{\omega}_{n-m}\Lambda^0_{ss'}(\omega)\operatorname{sgn} m.$$

The sum over m is expressed in terms of the logarithmic derivative of the gamma-function. Using its asymptotic form for large values of its argument, we find, with error $\sim(\pi T)^2/(\omega_n^2+\omega^2)$,

$$\pi T\sum_m\overline{\eta}^{\bullet}_{n-m}\operatorname{sgn} m=\omega\operatorname{arctg}\frac{\omega_n}{\omega}. \tag{17}$$

By means of formula (17) and the notation

$$\lambda_s^0(\omega)=\int\Lambda^0_{ss'}(\omega)\,d\tau_{s'},\quad \lambda_s^0=\int_0^\infty\lambda_s^0(\omega)\,d\omega^2,\quad \lambda_s=\frac{\lambda_s^0}{1+\lambda_s^0} \tag{18}$$

the quantity $|\omega_n+if_{ns}|$ is brought to the form

$$|\omega_n+if_{ns}|=|\omega_n|(1+\lambda_s^0)(1-\lambda_s q_{ns}), \tag{19}$$

where

$$q_{ns}=\int d\omega^2\frac{\lambda_s^0(\omega)}{\lambda_s^0}\left(1-\frac{\omega}{\omega_n}\operatorname{arctg}\frac{\omega_n}{\omega}\right). \tag{20}$$

The quantity λ_s^0 is the phonon renormalization of the electron mass at the point s on the Fermi surface. The function $\lambda_s q_{ns}$ describes the frequency dependence of the effective mass. In the entire region, $0<q_{ns}<1$; as $|\omega_n|\to 0$ we have $q_{ns}\sim\omega_n^2$; as $|\omega_n|\to\infty$ we obtain $q_{ns}\to 1$. The function $\omega^2\Lambda^0_{ss'}(\omega)$ generalizes the well-known function

$$\alpha^2(\omega)F(\omega)=\omega^2\int d\tau_s\,d\tau_{s'}\,\Lambda^0_{ss'}(\omega).$$

to the case of the anisotropic model.

Going over from the functions Φ_{ns} and χ_{0s} to the functions $\tilde{\Phi}_{ns}=a_s(1+\lambda_s^0)^{-1/2}\Phi_{ns}$ and $\tilde{\chi}_{0s}=a_s(1+\lambda_s^0)^{-1/2}\chi_{0s}$ and denoting

$$\begin{aligned}\Lambda^{\bullet}_{ss'}&=(1+\lambda_s^0)^{-1/2}\Lambda^0_{ss'}(\omega)(1+\lambda_{s'}^0)^{-1/2},\\ \tilde{\mu}^{\bullet}_{ss'}&=(1+\lambda_s^0)^{-1/2}\mu^{\bullet}_{ss'}(1+\lambda_{s'}^0)^{-1/2},\end{aligned} \tag{21}$$

we write Eqs. (8) and (14) in the following form:

$$\tilde{\Phi}_{ns}=\pi T\sum_m\int d\tau_{s'}\,d\omega^2\,\overline{\eta}^{\omega}_{n-m}\Lambda^{\omega}_{ss'}\frac{\tilde{\Phi}_{ms'}-\tilde{\chi}_{0s'}}{|\omega_m|(1-\lambda_{s'}q_{ms'})}, \tag{22}$$

$$\begin{aligned}\tilde{\chi}_{0s}=\pi T\sum_m\int d\tau_{s'}\,d\omega^2\,\tilde{\mu}^{\bullet}_{ss'}\Bigg[&\frac{\tilde{\Phi}_{ms'}-\overline{\eta}_m^{\omega}\tilde{\chi}_{0s'}}{|\omega_m|(1-\lambda_{s'}q_{ms'})}\\ &+\left(\frac{1}{1-\lambda_{s'}}-\frac{1}{1-\lambda_{s'}q_{ms'}}\right)\eta_m^{\omega}\tilde{\chi}_{0s'}\Bigg].\end{aligned} \tag{23}$$

2. CALCULATION OF T_c

The system of equations (22) and (23) can be solved by the perturbation method, if we note that, after expansion of the factor $(1-\lambda_{s'}q_{ms'})^{-1}$ in a geometric series, the right-hand sides of the equations will be series in powers of the electron-phonon interaction. The leading term of each such series contains, besides a first power of λ, a large logarithm that arises from the summation in the region of small $|\omega_m|$ and has the order of magnitude $\lambda\ln(\omega_D/T_c)\sim\lambda/(\lambda-\mu^*)\gtrsim 1$. The next term is of order $\sim\lambda^2$, since for this term the low-frequency region is cut off by the factor $q_{ms'}$. Our aim is to calculate, in the general case, the correction of order λ to the leading term, or, in other words, the leading correction to the BCS formula. Therefore, we shall put $q_{ms'}\equiv 0$, i.e., neglect the frequency dependence of the electron mass. In this approximation Eqs. (22) and (23) take the specially simple form:

$$\Phi_{ns}=\pi T\sum_m\overline{\eta}^{\omega}_{n-m}*\Lambda^{\omega}_{ss'}\cdot\frac{\Phi_{ms'}-\chi_{0s'}}{|\omega_m|}, \tag{24}$$

$$\chi_{0s}=\mu^{\bullet}_{ss'}\cdot\pi T\sum_m\frac{\Phi_{ms'}-\overline{\eta}_m^{\omega_0}\chi_{0s'}}{|\omega_m|}. \tag{25}$$

We have omitted the sign $\sim$ and, to abbreviate the formulas, have introduced the following notation for integrals over $d\omega^2$ and $d\tau_{s'}$:

$$\int X^{\omega}Y^{\omega}\,d\omega^2=X^{\omega}*Y^{\omega},\quad \int X_{ss'}Y_{s'}\,d\tau_{s'}=X_{ss'}\cdot Y_{s'}.$$

We shall separate out the logarithmic terms in the sums by means of a device proposed by Zubarev[16]. For this we write $\Phi_{ns}-\chi_{0s}$ in the form

$$\Phi_{ns}-\chi_{0s}=\delta_s-a_{ns}, \tag{26}$$

where δ_s is the boundary value of the function (26) on the Fermi surface. With regard to the function a_{ns}, we can assume that it depends on the continuous variable $\omega_n\to x$, and, in expressions containing a_{ms}, go over from sums to integrals. The error from this operation will change T_c by an amount of the order of $T_c(\pi T_c)^2/\omega_D^2$. By definition, the function a_{xs} satisfies the boundary condition $a_{0s}\equiv 0$. Substituting (26) into (24) and, as in (17), calculating

$$\pi T\sum_m\frac{\overline{\eta}^{\omega}_{n-m}}{|\omega_m|}=\overline{\eta}_n^{\omega}\left(\ln\frac{2\gamma\omega}{\pi T}+\ln\sqrt{1+(\omega_n/\omega)^2}+\frac{\omega_n}{\omega}\operatorname{arctg}\frac{\omega_n}{\omega}\right) \tag{27}$$

to within terms $\sim(\pi T_c)^2/(\omega_n^2+\omega^2)$, we obtain

$$\delta_s+\chi_{0s}=a_{xs}+\overline{\eta}_x^{\omega}\left(\ln\frac{2\gamma\omega}{\pi T}+\varphi_x^{\omega}\right)*\Lambda^{\bullet}_{ss'}\cdot\delta_{s'}-\int_{-\infty}^{+\infty}\frac{dy}{2y}\overline{\eta}^{\omega}_{x-y}*\Lambda^{\bullet}_{ss'}\cdot a_{ys'}. \tag{28}$$

Here we have changed to continuous variables and have denoted

$$\varphi_x^{\omega}=\ln\sqrt{1+(x/\omega)^2}+(x/\omega)\operatorname{arctg}(x/\omega);\quad \gamma=1.78\ldots$$

is the Euler constant.

Using Eq. (24) and formula (27) and writing $\ln(2\gamma\omega/\pi T_c)=\ln(2\gamma\omega_0/\pi T_c+\ln(\omega/\omega_0)$, we find (25), exact to the first two terms of the expansion in λ:

$$\chi_{0s}=\ln\left(\frac{2\gamma\omega_0}{\pi T_c}\right)\mu^{\bullet}_{ss'}\cdot\left(\delta_{s'}+\ln\frac{\omega}{\omega_0}*\Lambda^{\omega}_{s's_1}\cdot\delta_{s_1}\right). \tag{29}$$

We denote $E=\ln^{-1}(2\gamma\omega_0/\pi T_c)$ and substitute (29) into (28). As a result we obtain the equation

$$\begin{aligned}E\delta_s=&Ea_{xs}+\overline{\eta}_x^{\omega}*\Lambda^{\omega}_{ss'}\cdot\delta_{s'}-\mu^{\bullet}_{ss'}\cdot\delta_{s'}\\ &+E\left(\ln\frac{\omega}{\omega_0}+\varphi_x^{\omega}\right)*\Lambda^{\omega}_{ss'}\cdot\delta_{s'}-\mu^{\bullet}_{ss'}\cdot\ln\frac{\omega}{\omega_0}*\Lambda^{\omega}_{s's_1}\delta_{s_1}\\ &-E\int_{-\infty}^{\infty}\frac{dy}{2y}\overline{\eta}^{\omega}_{x-y}*\Lambda^{\omega}_{ss'}\cdot a_{ys'}.\end{aligned} \tag{30}$$

Assuming that E, λ and μ^* are of the same order, we find, in the first approximation,

$$E_0\delta_s^0=E_0a_{xs}^0+\overline{\eta}_x^{\omega}*\Lambda^{\omega}_{ss'}\cdot\delta_{s'}^0-\mu^{\bullet}_{ss'}\cdot\delta_{s'}^0. \tag{31}$$

For $x=0$, taking into account the boundary condition $a^0_{0s}\equiv 0$, we obtain the equation

$$E_0\delta_s^0=(\Lambda_{ss'}-\mu^{\bullet}_{ss'})\cdot\delta_{s'}^0,\quad \Lambda_{ss'}=\int\Lambda^{\omega}_{ss'}\,d\omega^2. \tag{32}$$

An equation of this type was obtained by Pokrovskiĭ[18] in 1961. The magnitude of T_c is determined by the maximum eigenvalue

$$E_0=\delta_s^0\cdot(\Lambda_{ss'}-\mu^{\bullet}_{ss'})\cdot\delta_{s'}^0=(\Lambda-\mu^*). \tag{33}$$

The brackets in the latter equality denote the average over the eigenfunction corresponding to E_0. Substituting (32) into (31), we obtain

$$E_0a_{xs}^0=\eta_x^{\omega}*\Lambda^{\omega}_{ss'}\cdot\delta_{s'}.$$

Writing out the second-approximation terms in (30) for $x=0$, we shall find the correction to E_0. Since $a^1_{0s}\equiv 0$,

$$E_1\delta_s^0+E_0\delta_s^1=(\Lambda_{ss'}-\mu^*_{ss'})\delta_{s'}^1+E_0\ln\frac{\omega}{\omega_0}*\Lambda^\omega_{ss'}\cdot\delta_{s'}^0$$

$$-\mu^*_{ss'}\cdot\ln\frac{\omega}{\omega_0}*\Lambda^\omega_{ss_1}\cdot\delta_{s_1}^0-\int_0^\infty\frac{dy}{y}\overline{\eta_y{}^\omega*\Lambda^\omega_{ss'}}\cdot\eta_y{}^{\omega'}*\Lambda^{\omega'}_{s's_1}\cdot\delta_{s_1}.$$

We shall denote the integral in the last term by

$$\int_0^\infty\frac{dy}{y}\overline{\eta_y{}^\omega}\,\eta_y{}^{\omega'}=\frac{1}{2}\frac{\omega^2}{\omega^2-\omega'^2}\ln\frac{\omega^2}{\omega'^2}=\frac{1}{2}A_{\omega\omega'}. \tag{34}$$

Since δ_S^1 is orthogonal to δ_S^0 and the kernel $\Lambda-\mu^*$ is symmetric, folding the latter equation with δ_S^0 we obtain

$$E_1=E_0\left(\ln\frac{\omega}{\omega_0}*\Lambda^\omega\right)-\left(\mu^*\ln\frac{\omega}{\omega_0}*\Lambda^\omega\right)-{}^1/_2(\Lambda^\omega*A_{\omega\omega'}*\Lambda^{\omega'}).$$

By defining the frequency ω_0 by the condition

$$\left(\ln\frac{\omega}{\omega_0}*\Lambda^\omega\right)=0, \tag{35}$$

we finally obtain

$$E=\ln^{-1}\frac{2\gamma\omega_0}{\pi T_c}=(\Lambda-\mu^*)-\left(\Lambda\ln\frac{\omega}{\omega_0}*\Lambda^\omega\right)-\frac{1}{2}(\Lambda^\omega*A_{\omega\omega'}*\Lambda^{\omega'}). \tag{36}$$

in the isotropic model,

$$\ln^{-1}\frac{2\gamma\omega_0}{\pi T_c}=\lambda-\mu^*-A\frac{\lambda^2}{2},\qquad A\lambda^2=\Lambda^\omega*A_{\omega\omega'}*\Lambda^{\omega'}. \tag{37}$$

We shall consider the case of weak anisotropy. We shall assume that the only source of the anisotropy is the phonon spectrum. We separate out the isotropic part in $\Lambda^0_{SS'}(\omega)$:

$$\Lambda^0(\omega)=\overline{\Lambda^0_{ss'}(\omega)}=\int\Lambda^0_{ss'}(\omega)\,d\tau_{s'},$$

so that

$$\Lambda^0_{ss'}(\omega)=\Lambda^0(\omega)+\zeta^0_{ss'}(\omega),\qquad \overline{\zeta^0_{ss'}(\omega)}\equiv 0. \tag{38}$$

Correspondingly,

$$\Lambda^*_{ss'}=\frac{\Lambda^\omega+\zeta^\omega_{ss'}}{\sqrt{(1+\zeta_s)(1+\zeta_{s'})}},\qquad \mu^*_{ss'}=\frac{\mu^*}{\sqrt{(1+\zeta_s)(1+\zeta_{s'})}}, \tag{39}$$

where

$$\Lambda^\omega=\Lambda^0(\omega)/(1+\lambda_0),\qquad \zeta^\omega_{ss'}=\zeta^0_{ss'}(\omega)/(1+\lambda_0),$$

$$\zeta_{ss'}=\int\zeta^\omega_{ss'}\,d\omega^2,\qquad \zeta_s=\int\zeta_{ss'}\,d\tau_{s'},\qquad \lambda_0=\int\Lambda^0(\omega)\,d\omega^2.$$

Substituting (39) into Eq. (32) and assuming ζ to be a small quantity, we find

$$E_0=\eta\left[1+\left(\frac{1-\eta}{\eta}\right)^2\overline{\zeta^2}\right],\qquad \delta_s^0=1+\frac{1-\eta}{\eta}\zeta_s,$$

$$\eta=\lambda-\mu^*,\qquad \overline{\zeta^2}=\int\zeta_s{}^2\,ds. \tag{40}$$

We recall that $\lambda=\lambda_0/(1+\lambda_0)$ is the renormalized average coupling constant and μ^* is also divided by $1+\lambda_0$; $\overline{\zeta^2}=\overline{(\Delta m)^2}/\overline{m}^2$ is the mean square deviation of the effective mass.

By means of the second formula in (40), we calculate the anisotropic correction to ω_0 and the last two terms in (36):

$$\Delta\omega_0=2\omega_0\frac{1-\eta}{\lambda\eta}\overline{\zeta_s\zeta_s{}^\omega}*\ln\frac{\omega}{\omega_0},$$

$$\left(\Lambda\ln\frac{\omega}{\omega_0}*\Lambda^\omega\right)=-\frac{\mu^*}{\eta}\overline{\zeta_s\zeta_s{}^\omega}*\ln\frac{\omega}{\omega_0},$$

$$(\Lambda^\omega*A_{\omega\omega'}*\Lambda^{\omega'})=\left(1-\frac{1-2\eta}{\eta^2}\overline{\zeta^2}\right)\Lambda^\omega*A_{\omega\omega'}*\Lambda^{\omega'}$$

$$+\left(\frac{1}{\eta}-2\right)\overline{\zeta_s\zeta_s{}^\omega}*(A_{\omega\omega'}+A_{\omega'\omega})*\Lambda^{\omega'}. \tag{41}$$

We shall give the formula for T_C for a model in which the frequency dependence of $\Lambda^\omega_{SS'}$ and the anisotropy are separated, i.e., $\Lambda^\omega_{SS'}=\Lambda^\omega(1+\lambda^{-1}\zeta_{SS'})$:

$$\ln^{-1}\frac{2\gamma\omega_0}{\pi T_c}=\eta-\frac{\lambda^2}{2}A+\frac{\overline{\zeta^2}}{\eta^2}\left[\eta(1-\eta)^2+(1-2\eta)^2\frac{\lambda^2}{2}A\right]. \tag{42}$$

In the general case, anisotropy facilitates the raising of T_C. In the BCS approximation this follows from Eq. (32), since, for the maximum eigenvalue E_0, the inequality

$$E_0>\overline{\Lambda_{ss'}-\mu^*_{ss'}}$$

is fulfilled.

As mentioned above, the general equations (22) and (23) can be solved by the perturbation method, the successive corrections to the solution being mutually related like $\lambda/(\lambda-\mu^*)$, λ, λ^2, ... For the simplest model with one Einstein mode it turns out to be possible to calculate the terms analytically to order λ^2. The frequency dependence of the mass makes an important contribution to these terms. We give the relevant result:

$$\ln^{-1}\frac{2\gamma\omega_0}{\pi T_c}=\lambda-\mu^*-\frac{\lambda^2}{2}+0.61\lambda^3-1.52\lambda^2\mu^*+0.65\lambda\mu^{*2}. \tag{43}$$

We shall consider a model with two phonon peaks ω_1 and ω_2. Let the coupling constants be determined by the expressions

$$\lambda_1{}^0=(\Omega/\omega_1)^2,\quad \lambda_2{}^0=(\Omega/\omega_2)^2,\quad \Omega\sim\omega_D. \tag{44}$$

In this model,

$$\Lambda^0(\omega)=\lambda_1{}^0\delta(\omega^2-\omega_1{}^2)+\lambda_2{}^0\delta(\omega^2-\omega_2{}^2),\quad \lambda_0=\lambda_1{}^0+\lambda_2{}^0.$$

From the condition (35) we determine the pre-exponential factor

$$\omega_0=\omega_1^{\lambda_1/(\lambda_1+\lambda_2)}\omega_2^{\lambda_2/(\lambda_1+\lambda_2)}. \tag{45}$$

Next we find

$$A=1+\frac{\rho\ln\rho}{\rho^2-1}-\frac{2\rho}{(1+\rho)^2},\qquad \rho=\frac{\lambda_1}{\lambda_2}=\frac{\omega_2{}^2}{\omega_1{}^2}. \tag{46}$$

For all ρ the quantity A differs little from unity and attains its maximum $A_{max}=1.066$ for $\rho\cong 0.1$.

3. EFFECT OF LOW-FREQUENCY PHONON PEAKS ON THE MAGNITUDE OF T_C

The question of the behavior of T_C in a model with two Einstein modes under the condition that the frequency ω_2 of one mode is fixed and the frequency ω_1 of the other tends to zero was considered in[10,11]. Expressions of the type (44) were used for the coupling constants, and T_C was calculated by means of the general formulas obtained by approximating the gap function by a step function[10] or by the Morel-Anderson function[11]. As a result T_C vanished as $\omega_1\to 0$. This physically incorrect result is easily reproduced using formulas (37), (44), (45) and (46). Since, for $\omega_1\to 0$, $\lambda_1^0\to\infty$ while $\lambda_2^0=$ const, we have $\omega_0\sim\omega_1$, $\lambda_1\to 1$, $\mu^*\to 0$, $A\to 1$. Therefore, for small ω_1, we have $T_C=1.14\,\omega_1\exp(-{}^2/_\lambda)$, so that $T_C(\omega_1\to 0)\to 0$. This behavior of $T_C(\omega_1)$ is connected with the fact that, in its calculation, for $Z(\omega)$ and $\Delta(\omega)$ approximations corresponding to the asymptotic behavior of these functions for $\omega_1\gg T_C$ were used. To obtain the correct result, it is necessary to calculate $f(\omega_n)$ and solve Eq. (7) without making the assumption that T_C is small compared to ω_1. We shall not touch upon the question of the dependence of the coupling constants on the frequencies for real systems, but, like the authors of[10,11], confine ourselves to a model with two Einstein peaks ω_1 and ω_2, with $\omega_2=$ const. We shall examine different power laws for the variable coupling constant λ_1^0:

$$\lambda_1{}^0=(\Omega/\omega_1)^{2-\nu},\quad 0<\nu<2,\quad \lambda_2{}^0=(\Omega/\omega_2)^2. \tag{47}$$

Qualitatively, the behavior of $T_C(\omega_1)$ as $\omega_1\to 0$ is very easily illustrated in the model with one peak ω in

the absence of the Coulomb interaction. In this case, formulas (5) and (2) take the form

$$\sigma_n = if_n/\pi T_c = \sum_m^{\text{odd}} \frac{\lambda^0\omega^2 \operatorname{sgn} m}{\omega^2_{n-m}+\omega^2}, \quad \Delta_n = \sum_m^{\text{odd}} \frac{\lambda^0\omega^2 \operatorname{sgn} m}{\omega^2_{n-m}+\omega^2} \frac{\Delta_m}{|m+\sigma_m|}. \quad (48)$$

We shall make the substitution $\tilde{\Delta}_n = \Delta_n/|n+\sigma_n|$ and in the equation for Δ_n carry over the term with $m = n$ into the left-hand side:

$$(|n+\sigma_n|-\lambda^0)\tilde{\Delta}_n = \lambda^0\omega^2 \sum_{m\neq n} \frac{\tilde{\Delta}_m}{\omega^2_{n-m}+\omega^2}. \quad (49)$$

Since

$$\sigma_n = \left(\lambda^0 + 2\lambda^0\omega^2 \sum_{k=2}^{|n|-1} \frac{1}{\omega^2_{n-m}+\omega^2}\right) \operatorname{sgn} n,$$

we see that λ_0 in the left-hand side of (49) is cancelled on account of σ_n. We denote $l = \omega/\pi T_c$ and $\lambda^0 l^2 = X$ and rewrite Eq. (49) with this notation:

$$\left(|n| + X\sum_{k=2}^{|n|-1} \frac{2}{k^2+l^2}\right)\tilde{\Delta}_n = X\sum_{m\neq n} \frac{\tilde{\Delta}_m}{(m-n)^2+l^2} \quad (50)$$

To each value of the parameter l corresponds a finite eigenvalue $X(l)$. As $l \to 0$ we have $X \to X_0 = \text{const}$, i.e., for small ω, $\lambda^0 l^2 \sim \text{const}$, whence it follows that $T_c \sim \omega^{\nu/2}$. Thus, for $\nu = 0$ we have $T_c \to \text{const} \neq 0$, while for $\nu > 0$ we obtain $T_c \to 0$. In exactly the same way it is easy to show that in the model (47) with two peaks, with or without the Coulomb interaction, the contribution to T_c from the soft mode ω_1 is always positive and for small ω_1 is proportional to ω_1^ν.

Figure 1 shows the results of the numerical solution

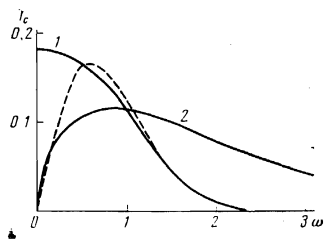

FIG. 1

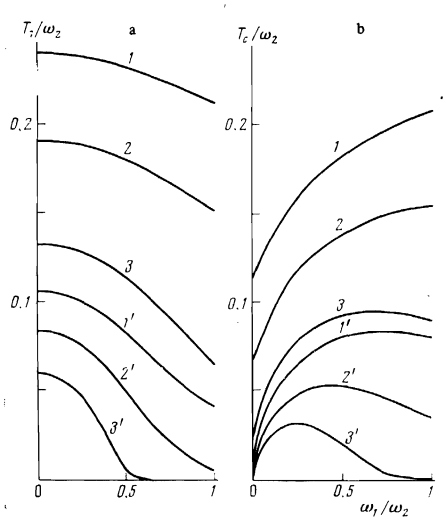

FIG. 2

of Eq. (50) for $\nu = 0$ (curve 1) and $\nu = 1$ (curve 2); the dashed curve corresponds to formula (43) with $\mu^* = 0$ and $\nu = 0$.

Figures 2a and 2b show the numerical results for the model with two peaks in the case $\nu = 0$ (Fig. 2a) and in the case $\nu = 1$ (Fig. 2b). All the frequencies and T_c are given in units of the scale frequency Ω. The curves 1, 2, and 3 correspond to $\omega_2 = 1$ ($\lambda_2^0 = 1$—strong coupling) and $\mu^* = 0$, 0.1 and 0.2. The curves 1′, 2′, and 3′ correspond to $\omega_2 = 2$ ($\lambda_2^0 = 0.25$—weak coupling) and $\mu^* = 0$, 0.1 and 0.2. In all cases the Coulomb pseudo-potential μ^* is defined not in terms of the average logarithmic frequency ω_0 but in terms of the scale frequency Ω.

We see that when an additional mode arises in the phonon spectrum of the superconductor, T_c increases in all cases; this is physically obvious, inasmuch as additional attraction betwen the electrons then appears. As this mode softens T_c increases monotonically, if the dependence of the coupling constant on frequency has the form $\lambda_1^0 \sim \omega_1^{-2}$. But if $\lambda_1 \sim \omega_1^{-2+\nu}$, where $\nu > 0$, then T_c first increases and then, passing through a maximum, falls, and for $\omega_1 = 0$ the contribution to T_c from the extra mode vanishes. The same result was obtained by Bergmann and Rainer[17], who considered the case $\lambda_1^0 = \text{const}$, i.e., $\nu = 2$.

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