Effect of the low-frequency peaks of the phonon state density on the critical temperature of superconductors

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A general expression for the critical superconducting transition temperature T_c is obtained on the basis of the Éliashberg equations for superconductors with strong coupling and by employing a simple approximation of the gap in the form of a steplike alternating function. It is shown that in the derivation of the familiar McMillan formula for T_c, some important renormalization terms containing an essential functional dependence of T_c on the shape of the phonon spectrum were either lost in the argument of the exponential function, or were incorrectly evaluated. Consequently the formula does not describe correctly the behavior of T_c in the presence of low-frequency peaks in the phonon state density. It is shown within the model of a phonon spectrum consisting of two Einstein peaks that upon decrease of frequency ω_1 of one of the peaks T_c passes through a maximum, and then decreases together with the effective coupling constant as $\omega_1 \to 0$. In other words, upon "softening" of the lattice (e.g., near the phase transition) T_c may not increase but rather decrease.

1. INTRODUCTION

At the present time, there have been a number of researches devoted to the effect of the features of the phonon spectrum of metals on the critical temperature of the superconducting transition T_c. In these works, the starting point for the analysis of the experimental results has usually been the well-known formula of McMillan:[1]

$$T_c = \frac{\Theta}{1.45} \exp\left[-\frac{1.04(1+\lambda)}{\lambda - \mu^*(1+0.62\lambda)} \right], \tag{1.1}$$

where λ is the constant of the electron-phonon interaction, μ^* the Coulomb "pseudopotential," and Θ the Debye temperature.

Equation (1.1) was obtained by McMillan in two stages. First, by means of a simple approximation of the gap by a step-like test function, which changes sign at the limiting frequency of the phonon spectrum ω_{max}, the equations of strong coupling theory were solved[2,3] as $T \to T_c$, and an approximate analytic expression was introduced for the critical temperature:[1]

$$T_c = \omega_{max} \exp\left[\frac{1+\lambda}{\lambda - \mu^* - (\langle\omega\rangle/\omega_{max})\lambda\mu^*} \right], \tag{1.2}$$

where

$$\langle\omega\rangle = \int_0^{\omega_{max}} d\omega\, \alpha^2(\omega) F(\omega) \Big/ \int_0^{\omega_{max}} \frac{d\omega}{\omega} \alpha^2(\omega) F(\omega); \tag{1.3}$$

$\alpha(\omega)$ is the characteristic function of the electron-phonon interaction, and $F(\omega)$ is the phonon state density. Then Eq. (1.2) was reconciled, by choosing the constant coefficients, with the results of the numerical solution of the equation for the gap, which was obtained by use of the phonon state density of niobium. It was assumed that $\alpha^2(\omega) = \text{const}$, and the contribution from the low-frequency region of the spectrum, as far as $\omega = 100°$ K, was not taken into account, i.e., it was implicitly assumed that all the phonon frequencies that are essential in $\alpha^2(\omega)F(\omega)$ satisfy the condition $\omega \gg T_c$.

However, it must be emphasized that some unjustified approximations were made in the derivation of Eq. (1.2), as a consequence of which there was an incorrect renormalization of the effective coupling constant. Therefore Eq. (1.1), which was used in [1] for the analysis of the experimental data, leads to incorrect empirical values of λ and μ^* and, as will be shown below, improperly describes the behavior of T_c when low-frequency branches appear in the phonon spectrum of superconductors.

Even in [1], an assumption was made which has far-reaching consequences. McMillan assumed that one could substitute the mean frequency $\langle\omega\rangle$ [Eq. (3)] as the pre-exponential factor in Eq. (1.1) in place of the Debye temperature Θ, so that the following relation is obtained for T_c in place of (1.1) for the case of niobium (see [4]):

$$T_c = \frac{\langle\omega\rangle}{1.20} \exp\left[-\frac{1.04(1+\lambda)}{\lambda - \mu^*(1+0.62\lambda)} \right]. \tag{1.4}$$

On the other hand, according to [1], the electron-phonon interaction constant can be represented in the form

$$\lambda = 2 \int_0^{\omega_{max}} \frac{d\omega}{\omega} \alpha^2(\omega) F(\omega) \approx \frac{\text{const}}{\langle\omega^2\rangle} \tag{1.5}$$

$$\langle\omega^2\rangle = \int_0^{\omega_{max}} d\omega\, \omega\alpha^2(\omega) F(\omega) \Big/ \int_0^{\omega_{max}} \frac{d\omega}{\omega} \alpha^2(\omega) F(\omega). \tag{1.6}$$

Starting from Eq. (1.4), and making the approximate substitution $\langle\omega^2\rangle \to \langle\omega\rangle^2$ in (1.5), McMillan showed[1] that T_c has a maximum as a function of $\langle\omega\rangle$, and calculated the values of T_c^{max} for various classes of superconducting materials.

Later, Dynes[4,5] analyzed a large number of experimental data and came to the conclusion that Eq. (1.4) much more accurately describes the dependence of T_c on the form of the function $\alpha^2(\omega)F(\omega)$ and on μ^* for various superconductors than Eq. (1.1). The reason for this will be made clear later on, and we note here only that the replacement of Θ in the pre-exponential factor by $\langle\omega\rangle$ has no rigorous justification.

In the present research, a simple approximation of the gap by an alternating-sign step function is used for the solution of the Éliashberg equations.[2] This function passes through zero at the point ω_0 (the frequency ω_0 is generally not equal to ω_{max}). As a result, a more accurate formula is obtained for the calculation of the critical temperature, which is valid in practice for any relation between T_c and the characteristic frequencies of the phonon spectrum, provided that ω_0 is much greater than T_c. It is shown that, within the framework of a model in which the phonon spectrum consists of two Einstein frequencies ω_1 and ω_2, when the frequency of at least one of the peaks of the phonon state density is decreased the critical temperature reaches a maximum and then falls off; the maximum value of T_c can be much lower than T_c^{max} computed from the formulas of McMillan.[1]

2. FORMULA FOR THE CRITICAL TEMPERATURE

We shall start out from the set of equations of Éliashberg[2] for superconductors with strong coupling as $T \to T_c$, with account taken of the Coulomb repulsion:

$$f_0(\omega) \equiv \omega[1-Z(\omega)] = \frac{1}{2}\int_0^\infty d\varepsilon \int_0^{\omega_{max}} d\nu\, \alpha^2(\nu)F(\nu)$$
$$\times\left\{\left[\operatorname{th}\left(\frac{\varepsilon}{2T_c}\right)+\operatorname{cth}\left(\frac{\nu}{2T_c}\right)\right]\left[\frac{P}{\varepsilon+\nu+\omega}-\frac{P}{\varepsilon+\nu-\omega}\right]\right.$$
$$\left.-\left[\operatorname{th}\left(\frac{\varepsilon}{2T_c}\right)-\operatorname{cth}\left(\frac{\nu}{2T_c}\right)\right]\left[\frac{P}{-\varepsilon+\nu+\omega}-\frac{P}{-\varepsilon+\nu-\omega}\right]\right\}; \quad (2.1)$$

$$C(\omega) = \frac{1}{2}Z^{-1}(\omega)\int_0^\infty \frac{d\varepsilon}{\varepsilon}C(\varepsilon)\int_0^{\omega_{max}} d\nu\,\alpha^2(\nu)F(\nu)$$
$$\times\left\{\left[\operatorname{th}\left(\frac{\varepsilon}{2T_c}\right)+\operatorname{cth}\left(\frac{\nu}{2T_c}\right)\right]\left[\frac{P}{\varepsilon+\nu+\omega}+\frac{P}{\varepsilon+\nu-\omega}\right]\right.$$
$$\left.+\left[\operatorname{th}\left(\frac{\varepsilon}{2T_c}\right)-\operatorname{cth}\left(\frac{\nu}{2T_c}\right)\right]\left[\frac{P}{-\varepsilon+\nu+\omega}+\frac{P}{-\varepsilon+\nu-\omega}\right]\right\}$$
$$-N(0)U_cZ^{-1}(\omega)\int_0 \frac{d\varepsilon}{\varepsilon}C(\varepsilon)\operatorname{th}\left(\frac{\varepsilon}{2T_c}\right). \quad (2.2)$$

Here N(0) is the normal density of the electron states at the Fermi level. $U_c = V_c[1+N(0)V_c\ln(E_F/\omega_c)]^{-1}$ is the intermediate Coulomb pseudopotential,[6] V_c is the matrix element of the screened Coulomb interaction, averaged over the Fermi surface, ω_c is the cutoff frequency, which lies in the range $\omega_{max} \ll \omega_c \ll E_F$, and E_F is the Fermi energy. (In writing down (2.1) and (2.2), just as in [1], we do not take into account attenuation effects, and all the integrals are taken in the sense of the principal value.)

If we replace $\coth(\nu/2T_0)$ in (2.2) by unity, which corresponds to a neglect of the thermal phonons, and set $\tanh(\epsilon/2T_c)=1$ in integrals which do not contain logarithmic singularities, then Eq. (2.2) is materially simplified (see [3]):

$$C(\omega) = Z^{-1}(\omega)\int_0^\infty \frac{d\varepsilon}{\varepsilon}C(\varepsilon)\operatorname{th}\left(\frac{\varepsilon}{2T_c}\right)\int_0^{\omega_{max}} d\nu\,\alpha^2(\nu)F(\nu)$$
$$\times\left[\frac{P}{\varepsilon+\nu+\omega}+\frac{P}{\varepsilon+\nu-\omega}\right]-N(0)U_cZ^{-1}(\omega)\int_0 \frac{d\varepsilon}{\varepsilon}C(\varepsilon)\operatorname{th}\left(\frac{\varepsilon}{2T_c}\right). \quad (2.3)$$

as $\omega \to 0$, Eq. (2.3) for the gap takes the form

$$C(0) = \frac{\lambda}{Z(0)}\int_0^\infty \frac{d\varepsilon}{\varepsilon}C(\varepsilon)\operatorname{th}\left(\frac{\varepsilon}{2T_c}\right)-\frac{2}{Z(0)}\int_0^{\omega_{max}}\frac{d\nu}{\nu}\alpha^2(\nu)F(\nu)\int_0^\infty\frac{d\varepsilon}{\varepsilon+\nu}C(\varepsilon)$$
$$-\frac{N(0)U_c}{Z(0)}\int_0^{\omega_c}\frac{d\varepsilon}{\varepsilon}C(\varepsilon)\operatorname{th}\left(\frac{\varepsilon}{2T_c}\right); \quad (2.4)$$

$$\lambda \equiv 2\int_0^{\omega_{max}}\frac{d\nu}{\nu}\alpha^2(\nu)F(\nu), \qquad Z(0) = \lim_{\omega\to 0}\left[1-\frac{f(\omega)}{\omega}\right] \quad (2.5)$$

At the same time, the asymptotic form of Eq. (2.3) as $\omega \to \infty$ is

$$C(\infty) = -\frac{N(0)U_c}{Z(\infty)}\int_0^{\omega_c}\frac{d\varepsilon}{\varepsilon}C(\varepsilon)\operatorname{th}\left(\frac{\varepsilon}{2T_c}\right). \quad (2.6)$$

By analogy with [1], we approximate the gap $C(\omega)$ by a step-like test function

$$C_t(\omega) = \begin{cases}\Delta_0, & 0<\omega<\omega_0\\ -\Delta_\infty, & \omega>\omega_0\end{cases}, \quad (2.7)$$

where the value of ω_0 is not yet specified,[1)] but it is assumed that the condition $\omega_0 \gg T_c$ is satisfied.

If we also set $\coth(\nu/2T_c) \approx \tanh(\epsilon/2T_c) \approx 1$ in (2.1) (the accuracy of such an approximation will be discussed in detail below, in Sec. 3), we then obtain the limiting relations for the normal self-energy part:

$$f_0(\omega) = \begin{cases}-\lambda\omega, & \omega\to 0 \quad (2.8a)\\ -\lambda\langle\nu^2\rangle/\omega, & \omega\to\infty \quad (2.8b)\end{cases},$$

where

$$\langle\nu^2\rangle \equiv \int_0^{\omega_{max}} d\nu\,\nu\alpha^2(\nu)F(\nu)\Big/\int_0^{\omega_{max}}\frac{d\nu}{\nu}\alpha^2(\nu)F(\nu). \quad (2.9)$$

Thus, in accord with (2.1) and (2.5), we have $Z(0)=1+\lambda$ and $Z(\infty)=1$.

As a result, we arrive at the following set of homogeneous linear equations relative to Δ_0 and Δ_∞ (cf. [1]):

$$(1+\lambda)\Delta_0 = \Delta_0\left[\lambda\ln\left(\frac{1.14\omega_0}{T_c}\right)-\lambda_0\right]-\Delta_\infty(1+\lambda_\infty); \quad (2.10)$$

$$\Delta_\infty = \Delta_0 N(0)U_c\ln\left(\frac{1.14\omega_0}{T_c}\right)-\Delta_\infty N(0)U_c\ln\left(\frac{\omega_c}{\omega_0}\right)$$
$$= \Delta_0\mu^*(\omega_0)\ln\left(\frac{1.14\omega_0}{T_c}\right), \quad (2.11)$$

where

$$\mu^* = \frac{N(0)U_c}{1+N(0)U_c\ln(\omega_c/\omega_0)} \equiv \frac{N(0)V_c}{1+N(0)V_c\ln(E_F/\omega_0)}; \quad (2.12)$$

$$\lambda_0 = 2\int_0^{\omega_{max}}\frac{d\nu}{\nu}\alpha^2(\nu)F(\nu)\ln\left(1+\frac{\omega_0}{\nu}\right), \quad (2.13)$$

$$\lambda_\infty = 2\int_0^{\omega_{max}}\frac{d\nu}{\nu}\alpha^2(\nu)F(\nu)\ln\left(1+\frac{\nu}{\omega_0}\right). \quad (2.14)$$

From the condition of solvability of the set (2.10) and (2.11), we obtain an exponential formula for the critical temperature of the superconducting transition:

$$T_c = 1.14\omega_0\exp\left[-\frac{1+\lambda+\lambda_0}{\lambda-\mu^*(1+\lambda_\infty)}\right]. \quad (2.15)$$

Comparing (2.15) with the results of McMillan,[1] we see that the argument of the exponential of (1.2) does not contain the term λ_0,[2)] and the quantity $\langle\omega\rangle\lambda/\omega_{max}$ is obtained from λ_∞ under the condition $\omega_0 = \omega_{max} \gg \nu$ with account taken of only the first term in the expansion of the logarithm under the integral sign in (2.14). The absence of λ_0 in (1.2) (or in (1.1)) corresponds to the neglect of the effects of retardation of the electron-phonon interaction in the most important region of energies $0<\epsilon<\omega_0$, i.e., to the substitution of a constant for the kernel of the integral equation (2.3) in this region. As we shall see, this is entirely invalid even in the case in which all the characteristic frequencies of the phonon spectrum are much greater than T_c, inasmuch as λ_0 is a quantity of the same order as λ. If there are low-frequency peaks in the phonon state density, then the term λ_0 becomes dominant, and the value of T_c is essentially determined by the ratio λ_0/λ.

Up to this point, we have not specified the quantity ω_0, in the choice of which there is considerable leeway. Thus, for example, we can set $\omega_0=\omega_{max}$, as is done in [1,7]. However, it is more natural to define, in accord with (2.7), the quantity ω_0, as the point when the sign of the gap reverses, where $C(\omega_0)=0$. Then we get from (2.3) the following equation for finding ω_0:

$$\int_0^\infty \frac{d\varepsilon}{\varepsilon} C(\varepsilon)\,\mathrm{th}\left(\frac{\varepsilon}{2T_c}\right) \int_0^{\omega_{max}} d\nu\, \alpha^2(\nu)F(\nu) \left[\frac{P}{\varepsilon+\nu+\omega_0}+\frac{P}{\varepsilon+\nu-\omega_0}\right] = N(0)U_c \int_0^{\omega_c} \frac{d\varepsilon}{\varepsilon} C(\varepsilon)\,\mathrm{th}\left(\frac{\varepsilon}{2T_c}\right). \qquad (2.16)$$

Unfortunately, it is not possible to find self-consistent solutions of Eq. (2.16) within the framework of the simplest approximation (2.7). However, the frequency ω_0 can be estimated approximately if we use the method of Zubarev[8] and choose as the first iteration for the gap $C(\omega)$ the kernel of the integral equation (2.3), taken at the point $\epsilon=0$. Then ω_0 is determined from the condition

$$\int_0 d\nu\, \alpha^2(\nu)F(\nu) \left[\frac{P}{\nu+\omega_0}+\frac{P}{\nu-\omega_0}\right] - \mu^*(\omega_0) = 0. \qquad (2.17)$$

(For the estimate, we can limit ourselves to qualitative consideration of the Coulomb interaction of the electrons, introducing the true pseudopotential μ^* in the last term of Eq. (2.3) by cutting off the upper limit of the integration at the frequency ω_0.) It is easy to see that when so determined, the frequency ω_0 never vanishes, although it depends essentially on the shape of the phonon spectrum (roughly speaking, ω_0 lies close to the "center of gravity" of the function $\alpha^2(\nu)F(\nu)$).

Finally, we note that the expression (2.15) can formally be represented as

$$T_c = 1.14\tilde{\omega} \exp\left[-\frac{1+\lambda}{\lambda-\mu^*(1+\lambda_\infty)}\right], \qquad (2.18)$$

where

$$\tilde{\omega} = \omega_0 \exp\left[-\frac{\lambda_0}{\lambda-\mu^*(1+\lambda_\infty)}\right]. \qquad (2.19)$$

In this notation, the argument of the exponential in (2.18) becomes much closer to those in formulas (1.1), (1.2) or (1.4) of McMillan; however, the pseudopotential factor $\tilde{\omega}$ is materially different from Θ, ω_{max} or $\langle\omega\rangle$.

3. FORMULA FOR THE CRITICAL TEMPERATURE IN THE PRESENCE OF LOW-FREQUENCY SINGULARITIES IN THE PHONON SPECTRUM

The case of the existence of low-frequency peaks in the phonon spectrum[3)] requires special consideration, inasmuch as it is impossible to set $\tanh(\epsilon/2T_c) = \coth(\nu/2T_c) = 1$ beforehand in Eq. (2.1), and also to use for the gap the simplified equation (2.3) in place of the exact equation (2.2).

We first consider the expression (2.1) for the normal self-energy part $f_0(\omega)$. It is easy to show that the terms proportional to $\coth(\nu/2T_c)$, do not make a contribution to $f_0(\omega)$ in integration with respect to ϵ from 0 to ∞. Therefore (2.1) can be transformed to

$$f_0(\omega) = \int_0^\infty dx\, x\,\mathrm{th}\,x \int_0^{\omega_{max}} d\nu\, \alpha^2(\nu)F(\nu) \left[\frac{P}{x^2-\nu_+^2}-\frac{P}{x^2-\nu_-^2}\right]$$

$$= -\frac{1}{2} P\int_0^\infty \frac{dx}{\mathrm{ch}^2 x} \int_0^{\omega_{max}} d\nu\, \alpha^2(\nu)F(\nu) \ln\left|\frac{x^2-\nu_+^2}{x^2-\nu_-^2}\right|, \qquad (3.1)$$

$$\nu_\pm = (\nu\pm\omega)/2T_c.$$

Integration with respect to x in (3.1) can be carried out exactly if we consider the following relation (see the Appendix)

$$P\int_0^\infty \frac{dx}{\mathrm{ch}^2 x} \ln|x^2-\nu_\pm^2| = 2\left[\ln\pi + \mathrm{Re}\,\psi\left(\frac{1}{2}+i\frac{\nu_\pm}{\pi}\right)\right], \qquad (3.2)$$

where ψ is the logarithmic derivative of the Γ function. As a result, we get for $f_0(\omega)$

$$f_0(\omega) = -\int_0^{\omega_{max}} d\nu\, \alpha^2(\nu)F(\nu) \left[\mathrm{Re}\,\psi\left(\frac{1}{2}+i\frac{\nu_+}{\pi}\right) - \mathrm{Re}\,\psi\left(\frac{1}{2}+i\frac{\nu_-}{\pi}\right)\right]. \qquad (3.3)$$

It then follows that as $\omega\to 0$ the function takes the form

$$f_0(\omega) \cong -\omega\left[-\frac{\partial f_0(\omega)}{\partial\omega}\right]_{\omega=0} = -\omega\Lambda(T_c), \qquad (3.4)$$

where

$$\Lambda(T_c) = -\frac{1}{\pi T_c}\int_0 d\nu\, \alpha^2(\nu)F(\nu)\,\mathrm{Im}\,\psi'\left(\frac{1}{2}+i\frac{\nu}{2\pi T_c}\right) \qquad (3.5)$$

(here ψ' is the first derivative of the ψ function). Under the condition $\nu \gg \pi T_c$, we can make use of the well-known asymptotic form (see [10])

$$\mathrm{Im}\,\psi'\left(\frac{1}{2}+i\frac{\nu}{2\pi T_c}\right) \approx -\frac{2\pi T_c}{\nu} + O\left(\left[\frac{2\pi T_c}{\nu}\right]^3\right), \qquad (3.6)$$

by virtue of which we obtain $\Lambda(T_c)\approx\lambda$, so that (3.4) goes over into the relation (2.8a).

In the range of energies $\omega \gg \omega_0$, the following asymptotic expansion is valid (see [10]):

$$\mathrm{Re}\,\psi\left(\frac{1}{2}+i\frac{\nu_\pm}{\pi}\right) \approx \ln\left(\frac{\omega}{2\pi T_c}\right) \pm \frac{\nu}{\omega} + O\left(\left[\frac{\nu}{\omega}\right]^2\right), \qquad (3.7)$$

whence it is seen that the expression (3.3) reduces to (2.8b) in this limiting case.

We now concern ourselves with the solution of the exact equation for the gap (2.2). If we stay as before within the framework of approximations (2.7) for $C(\omega)$, then in the limit of small ν particular attention must be paid to the calculation of the integration of terms containing $\tanh(\epsilon/2T_c)$ with respect to ϵ in the range $0<\epsilon<\omega_0$.

$$P\int_0^{\omega_0} d\varepsilon\left(\frac{1}{\varepsilon}+\frac{\varepsilon}{\nu^2-\varepsilon^2}\right)\mathrm{th}\left(\frac{\varepsilon}{2T_c}\right)$$

$$\cong \ln\left(\frac{\omega_0}{2T_c}\right) - \frac{1}{2}\ln\left|\frac{\omega_0^2-\nu^2}{(2T_c)^2}\right| - \int_0^\infty \frac{dx}{\mathrm{ch}^2 x}\ln x \qquad (3.8)$$

$$+\frac{1}{2}P\int_0^\infty \frac{dx}{\mathrm{ch}^2 x}\ln\left|x^2-\left(\frac{\nu}{2T_c}\right)^2\right|.$$

(Here the upper limit $\omega_0/2T_c \gg 1$ is replaced approximately by ∞.)

Carrying out calculations similar to those that led to Eq. (2.15), in Sec. 2, with account taken of the relation (3.2), we get the following transcendental equation for T_c:

$$T_c = 1.14\omega_0 \exp\left\{-\frac{1+\Lambda(T_c)+\Lambda_0(T_c)}{\lambda-\mu^*[1+\Lambda_\infty(T_c)]}\right\}, \qquad (3.9)$$

where

$$\Lambda_0(T_c) = \int_0^{\omega_{max}} \frac{d\nu}{\nu}\alpha^2(\nu)F(\nu)\left\{\ln\left|1-\frac{\omega_0^2}{\nu^2}\right| + 2\ln\left(\frac{\nu}{2\pi T_c}\right) - 2\,\mathrm{Re}\,\psi\left(\frac{1}{2}+i\frac{\nu}{2\pi T_c}\right) + \ln\left|\frac{\omega_0+\nu}{\omega_0-\nu}\right|\mathrm{cth}\left(\frac{\nu}{2T_c}\right)\right\}; \qquad (3.10)$$

$$\Lambda_\infty(T_c) = \int_0^{\omega_{max}} \frac{d\nu}{\nu}\alpha^2(\nu)F(\nu)\left\{\ln\left|1-\frac{\nu^2}{\omega_0^2}\right| + \ln\left|\frac{\omega_0+\nu}{\omega_0-\nu}\right|\mathrm{cth}\left(\frac{\nu}{2T_c}\right)\right\}. \qquad (3.11)$$

Under the condition $\nu/\pi T_c \gg 1$, the quantity $\Lambda_0(T_c)$ goes over into λ_0, and $\Lambda_\infty(T_c)$ is identical with λ_∞, i.e., Eq. (3.9) reduces to Eq. (2.15).

4. CRITICAL TEMPERATURE IN THE PHONON SPECTRUM MODEL WITH TWO EINSTEIN PEAKS

The calculation of T_c from Eq. (2.15) or (3.9) can be carried out only in the case in which the explicit dependence of the function $\alpha^2(\nu)F(\nu)$ on ν is known. In the general case, this function is of the form[1]

$$\alpha^2(\nu)F(\nu)=\int\limits_{S_F}\frac{d^2k}{v_F}\int\limits_{S_F'}\frac{d^2k'}{v_F'(2\pi)^3}\sum_j M^2_{\mathbf{kk}',j}\delta(\nu-\omega_{\mathbf{k}-\mathbf{k}',j})\Big/\int\limits_{S_F}\frac{d^2k}{v_F}, \quad (4.1)$$

where $M_{\mathbf{kk}',j}=(2MN\omega_{\mathbf{k}-\mathbf{k}',j})^{-1/2}g_j(\mathbf{k},\mathbf{k}')$ is the matrix element of the electron-phonon interaction, $g_j(\mathbf{k},\mathbf{k}')=\langle\mathbf{k}|\mathbf{e}_{\mathbf{k}-\mathbf{k}',j}\nabla U|\mathbf{k}'\rangle$ is the matrix element of the electron-ion interaction, $\omega_{\mathbf{k}-\mathbf{k}',j}$ and $\mathbf{e}_{\mathbf{k}-\mathbf{k}',j}$ are the frequency and polarization vector of a phonon with momentum $\mathbf{k}-\mathbf{k}'$ and polarization j, and v_F is the Fermi velocity of the electrons (integration in (4.1) is carried out over the Fermi surface). As was shown in [1], the first moment of the function $\alpha^2(\nu)F(\nu)$ does not depend on the phonon frequencies:

$$\int\limits_0^{\omega_{max}}d\nu\,\nu\alpha^2(\nu)F(\nu)=\frac{N(0)}{2M}\sum_j\langle g_j^2\rangle=\text{const.} \quad (4.2)$$

To analyze the behavior of T_c when the low-frequency peaks appear in the phonon state density, we choose a simple spectrum model in the form of two Einstein frequencies (cf. with [6,12]):

$$\alpha^2(\nu)F(\nu)=\sum_{i=1}^{2}\alpha_i^2(\nu)\frac{\Gamma_i/\pi}{(\nu-\omega_i)^2+\Gamma_i^2}\approx\sum_{i=1}^{2}\alpha_i^2(\nu)\delta(\nu-\omega_i) \quad (4.3)$$

(the latter is valid under the condition $\omega_i\gg\Gamma_i$, where Γ_i is the width of the peak). In this case, in contrast to [6] (see also [1]), we consider in (4.3) the dependence of $\alpha^2(\nu)$ on ν, which is especially important in the presence of low-frequency peaks.[4)] We note that the approximation $\alpha_i^2(\nu)=\text{const}$, made in [6], does not allow us to satisfy the exact condition (4.2).

Within the framework of the Einstein spectrum model, we have, in accord with (4.1),

$$\alpha_i^2(\nu)=\frac{1}{2}\beta\omega_{max}^2\frac{\eta_i}{\nu},\qquad\sum_{i=1}^{2}\eta_i=1. \quad (4.4)$$

Calculating the first moment of Eq. (4.3), with allowance for (4.4), and comparing it with (4.2), we find the dimensionless parameter β:

$$\beta=\frac{N(0)}{M\omega_{max}}\sum_j\langle g_j^2\rangle. \quad (4.5)$$

With the help of the relations (4.3) and (4.4), we can reduce the parameters λ, λ_0, λ_∞, which appear in Eq. (2.15), to the following form:

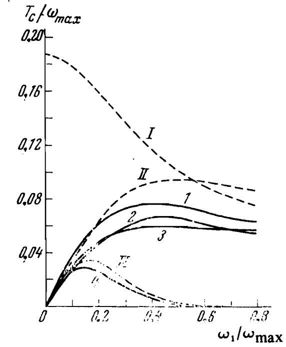
$$\lambda=\sum_{i=1}^{2}\lambda_i=\beta\sum_{i=1}^{2}\eta_i\left(\frac{\omega_{max}}{\omega_i}\right)^2,$$

$$\lambda_0=\beta\sum_{i=1}^{2}\eta_i\left(\frac{\omega_{max}}{\omega_i}\right)^2\ln\left|1+\frac{\omega_0}{\omega_i}\right|, \quad (4.6)$$

$$\lambda_\infty=\beta\sum_{i=1}^{2}\eta_i\left(\frac{\omega_{max}}{\omega_i}\right)^2\ln\left|1+\frac{\omega_i}{\omega_0}\right|.$$

The quantities Λ, Λ_0 and Λ_∞, which appear in Eq. (3.9), can be represented in similar fashion.

Greatest interest attaches to the problem of the effect of the location of the peak of the phonon state density in the low-frequency region on the temperature of the superconducting transition. With this aim in view, the value of T_c/ω_{max} was calculated from Eqs. (2.15) and (3.9) for the Einstein spectrum (4.3) as a function



Dependence of T_c/ω_{max} on ω_1/ω_{max}, calculated in various approximations for $\omega_2/\omega_{max}=0.8$ and $\eta_1=0.3$. The curves 1 and 2 were computed in accord with Eqs. (2.15) and (3.9), respectively for $\beta=1$ with $\omega_0=\omega_{max}$, while curves 3 and 4 were done in accord with Eq. (2.15) for $\beta=1$ and $\beta=0.2$ respectively, with ω_0 from (2.17). Curve I is computed from Eq. (1.1) at $\beta=1$, and curves II and III, from Eq. (1.4) at $\beta=1$ and $\beta=0.2$, respectively.

of the ratio ω_1/ω_{max} for various values of the parameters β, ω_0, ω_2 and η_1 (the coefficient η_2 is determined from the normalization condition: $\eta_1+\eta_2=1$) and for $\mu^*(\omega_{max})=0.13$ (here $\mu^*(\omega_{max})$ is the value of the Coulomb pseudo-potential at $\omega_0=\omega_{max}$).

The figure shows the results of the calculation of T_c/ω_{max} as a function of ω_1/ω_{max} for $\omega_2/\omega_{max}=0.8$ and $\eta_1=0.3$. Curves 1 and 2 were plotted from Eqs. (2.15) and (3.9), respectively, for the case $\beta=1$ and at the fixed frequency $\omega_0=\omega_{max}$, while curves 3 and 4 were computed from Eq. (2.15) for $\beta=1$ and $\beta=0.2$, respectively, with a "floating" pre-exponential factor ω_0 determined from Eq. (2.17) and dependent on the location of the peak ω_1/ω_{max}. It is seen that as ω_1/ω_{max} decreases all the T_c/ω_{max} curves pass through a maximum (the temperature corrections, made with use of Eq. (3.9), and the corrections associated with improved choice of the pre-exponential factor in accord with (2.17), are not always small and in a number of cases, lead to a considerable reduction in the maximum value of the ratio T_c/ω_{max}).

For comparison, the figure shows curves I and II calculated from Eqs. (1.1) and (1.4), respectively, for the same values of the parameters ($\beta=1$, $\mu^*=0.13$, $\omega_2/\omega_{max}=0.8$ and $\eta_1=0.3$) and with use of the ratio $\omega/\omega_{max}=0.84$ for niobium, and also curve III, calculated from (1.4) for $\beta=0.2$. As we see, the behavior of curve I in the range of small ω_1/ω_{max} differs significantly from the behavior of curves 1–3.

Thus, in the presence of low-frequency peaks in the phonon spectrum of the superconductor, Eq. (1.1) with a constant pre-exponential factor Θ certainly yields incorrect results. At the same time, curves II and III are qualitatively correct plots of the dependence of T_c/ω_{max} on ω_1/ω_{max} for the simple reason that the mean frequency $\langle\omega\rangle$ introduced in [1], which is defined by the relation (1.3) and which enters as a pre-exponential factor in (1.4), tends to zero as $\omega_1/\omega_{max}\to 0$ for the phonon spectrum model (4.3) under consideration.[5)] The much better agreement of Eq. (1.4) with experiment (in comparison with Eq. (1.1)), already noted in [4,5], is connected with just this rather fortuitous circumstance. Nevertheless, the region of applicability of Eq. (1.4) is very limited, since it is obtained from (1.1) by simple replacement of $\Theta/1.45$ by $\langle\omega\rangle/1.20$ in the pre-exponential factor; this replacement is valid only for the phonon spectrum of niobium. Moreover, in (1.4), just as in the original formula (1.1) of McMillan, the term λ_0, which depends materially on the shape of the function $\alpha^2(\nu)F(\nu)$, is in practice lost from the argument of the exponential (the coefficient 1.04 cannot compensate for the absence of $\lambda_0\gtrsim\lambda$) and the term λ_∞ is replaced by the constant 0.62λ (see (2.15)). Therefore, in the case of superconductors for which the essential role is played by the interaction of electrons with low-frequency phonons, Eq. (1.4) leads to an overestimate of T_c (see, for example, curves II and 2 of the figure), although in the weak coupling limit, when $\beta \ll 1$, this error can be small (see curves III and 4 in the drawing).

5. CONCLUSION

In the previous sections, expressions were obtained for the determination of the critical temperature of the superconducting transition T_c on the basis of the Éliashberg equations[2] for superconductors with strong coupling and with the help of a simple approximation of the gap $C(\omega)$ by a step-like alternating function (see Eqs. (2.15) and (3.9)). These equations depend on the form of the function $\alpha^2(\nu)F(\nu)$ that characterizes the intensity of the electron-phonon interaction, and on the value of the averaged screened Coulomb interaction between the electrons $N(0)V_c$, which enters via the pseudopotential μ^*.

In Sec. 4, these general expressions were analyzed for the particular model of a phonon spectrum in the shape of two Einstein branches and it was shown that the appearance of a sharp peak in the function $\alpha^2(\nu)F(\nu)$ in the low frequency region $\nu \ll \omega_{max}$ does not lead to an increase in T_c in all cases but only at a definite ratio of the parameters. If we consider the dependence of T_c only on the location of the low-frequency peak ω_1 in the phonon spectrum, disregarding, for simplicity, any change in the other parameters of the problem, then it turns out that in the final analysis, the shift of this peak to zero frequency[6)] leads to a weakening of the superconductivity. This result casts doubts on the widespread opinion that "softening" of the lattice always leads to an increase in T_c, and that such an increase is limited only by the loss of stability of the crystal lattice. Of course, for the final settlement of this question, we need to study other, more realistic models of the phonon spectrum with a smooth accumulation of phonons in the region of low frequencies, and also to study the effect of such factors as the width of the peak, the damping of the phonons as a consequence of anharmonicity, and so on.

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APPENDIX

In theoretical papers on superconductivity, one frequently encounters the integral

$$P\int_0^\infty \frac{dx}{\mathrm{ch}^2 x}\ln|x^2-a^2|,$$

however, so far as we know, it has not yet been computed exactly. For the calculation of this integral, we represent it in the form of a sum:

$$P\int_0^\infty \frac{dx}{\mathrm{ch}^2 x}\ln|x^2-a^2| = 2\int_0^\infty \frac{dx}{\mathrm{ch}^2 x}\ln x + \frac{1}{2}P\int_{-\infty}^\infty \frac{dx}{\mathrm{ch}^2 x}\ln\left|1-\frac{a^2}{x^2}\right|. \quad (A.1)$$

The first of these integrals is equal to (see [11])

$$\int_0^\infty \frac{dx}{\mathrm{ch}^2 x}\ln x = \ln\pi + \psi\left(\frac{1}{2}\right). \quad (A.2)$$

The second integral can be calculated by means of a contour that is closed in the upper half-plane, since the integral over the large semicircle approaches zero:

$$\left|\int_{C_R}\frac{dz}{\mathrm{ch}^2 z}\ln\left|1-\frac{a^2}{z^2}\right|\right| \leqslant \left|\int_{C_R} dz\ln\left|1-\frac{a^2}{z^2}\right|\right| \leqslant \pi R\ln\left|1+\frac{a^2}{R^2}\right| \underset{R\to\infty}{\to} 0. \quad (A.3)$$

The integrals over the semicircles of small radius $r \to 0$ around the points $z=0, \pm a$ also approach zero. Then the residues at the poles of second order $z = i(n+1/2)\pi$ give

$$P\int_{-\infty}^\infty \frac{dx}{\mathrm{ch}^2 x}\ln\left|1-\frac{a^2}{x^2}\right| = \oint\frac{dz}{\mathrm{ch}^2 z}\ln\left|1-\frac{a^2}{z^2}\right|$$
$$= -2\sum_{n=0}^\infty\left(\frac{1}{n+1/2+ia/\pi}+\frac{1}{n+1/2-ia/\pi}-\frac{2}{n+1/2}\right) \quad (A.4)$$
$$= 2\left[\psi\left(\frac{1}{2}+i\frac{a}{\pi}\right)+\psi\left(\frac{1}{2}-i\frac{a}{\pi}\right)-2\psi\left(\frac{1}{2}\right)\right],$$

whence it follows with account of (A.2) that

$$P\int_0^\infty \frac{dx}{\mathrm{ch}^2 x}\ln|x^2-a^2| = 2\ln\pi + \psi\left(\frac{1}{2}+i\frac{a}{\pi}\right)$$
$$+\psi\left(\frac{1}{2}-i\frac{a}{\pi}\right) = 2\left[\ln\pi + \mathrm{Re}\,\psi\left(\frac{1}{2}+i\frac{a}{\pi}\right)\right]. \quad (A.5)$$

Note added in proof, July 27, 1973. Recently, we were made aware of the work of Allen (P. B. Allen, Solid St. Commun. 12, 379 (1973)), in which arguments concerning the negative effect of low-frequency phonons on superconductivity are also advanced.

1) To avoid confusion, we note that in [1] the limiting frequency of the phonons was denoted by ω_0. Here, in the general case, $\omega_0 \neq \omega_{max}$.

2) Evidently, the existence of the term λ_0 in the argument of the exponential was first noted by Leavens and Carbotte; [7] however, without any justification, they cut off the interaction of the electrons with the phonons at the frequency $\omega = \omega_{max}$ (the limiting frequency of the phonons ω_{max} was denoted by ω_c in [7]). Because of this, they lost the Coulomb-pseudopotential renormalization determined by λ_∞.

3) Anomalies in the tunnel density of states in Nb_2Sn were experimentally observed [9] in the frequency range $\nu \sim (2\text{-}4)T_c$.

4) It was assumed in [12] that $\omega_i \gg T_c$, and only the temperature corrections $\sim(T_c/\omega_i)^2$ were taken into account.

5) We note that with the help of the relations (3.18) and (2.19) one can also regard the decrease of T_c as $\omega_1 \to 0$ formally as the result of the approach of the pre-exponential factor $\tilde{\omega}$ to zero. However, the physical meaning of the falloff in T_c upon appearance of low-frequency peaks in the phonon state density lies in the decrease of the effective coupling constant $\lambda_{eff} = [\lambda - \mu^*(1+\lambda_\infty)]/(1+\lambda+\lambda_0)$.

6) Such a situation can take place, in particular, close to a phase transition of the lattice from one crystalline modification to another.

[1] W. L. McMillan, Phys. Rev. 167, 331 (1968).
[2] G. M. Éliashberg, Zh. Eksp. Teor. Fiz. 39, 1437 (1960) [Soviet Phys.-JETP 12, 1000 (1961)].
[3] V. Ambegaokar and L. Tewordt, Phys. Rev. 134, A805 (1964).
[4] R. C. Dynes, Phys. Rev. B2, 644 (1970).
[5] R. C. Dynes, Solid. St. Commun. 10, 615 (1972).
[6] D. J. Scalapino, J. R. Schrieffer and J. W. Wilkins, Phys. Rev. 148, 263 (1966).
[7] C. R. Leavens and J. P. Carbotte, Canad. J. Phys. 49, 724 (1971).
[8] D. N. Zubarev, Usp. Fiz. Nauk, 71, 71 (1960) [Soviet Phys.-Uspekhi 3, 320 (1960)].
[9] S. I. Vedeneev, A. I. Golovashkin and G. P. Motulevich,

ZhETF Pis. Red. 16, 216 (1972) [JETP Lett. 16, 152 (1972)].
[10]Tables of Logarithmic Derivatives of the Gamma Function and its Derivatives in Complex Plane (in Russian). Computation Center, Academy of Sciences USSR, 1965.
[11]I. S. Gradshteĭn and I. M. Ryzhik, Tablitsy integralov, summ, syadov i proizvedenii, (Tables of Integrals, Sums, Series and Products) Fizmatgiz, 1963.
[12]B. T. Geĭlikman and N. F. Masharov, J. Low. Temp. Phys. 6, 131 (1972).

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