Effect of the frequency dependence of the electron-phonon interaction spectral function on the thermodynamic properties of superconductors

A. E. Karakozov, E. G. Maksimov, and S. A. Mashkov

P. N. Lebedev Physics Institute, USSR Academy of Sciences
and Institute of High Pressure Physics, USSR Academy of Sciences
(Submitted December 12, 1974)
Zh. Eksp. Teor. Fiz. **68**, 1937–1950 (May 1975)

The thermodynamic properties of superconductors are investigated. It is shown that the electron density of states in real superconductors does not vanish anywhere, owing to the decay caused by interaction between Cooper pairs and thermal phonons. It is noted that this effect is similar to the influence of magnetic impurities. In contrast to the latter, however, it does not lead to a lowering of T_c. Aproximate formulas for T_c are derived and compared with the familiar McMillan formulas. The range of applicability of the formulas is established by comparing them with the exact numerical solution of the Éliashberg equations. The dependence of T_c on the form and position of the phonon density of states is investigated. It is shown that the increase of T_c due to the softening of the phonon spectra is possible only when the electron coupling constant increases.

PACS numbers: 74.20.Ef

1. INTRODUCTION

It is well known that the thermodynamic properties of practically all the presently existing superconductors are determined mainly by the electron-phonon interaction. The direct Coulomb interelectron repulsion on account of the effect of the logarithmic attenuation due to rescattering of the electrons far from the Fermi surface is strongly suppressed and exerts a very small influence on the entire thermodynamics of the superconducting state.

The main characteristic of the electron-phonon interaction is the spectral function $S(\omega) \equiv \alpha^2(\omega)g(\omega)$[1], where $g(\omega)$ is the phonon density of states and $\alpha^2(\omega)$ are the coupling constants of the electrons with phonons of given energy ω. Knowledge of the matrix elements of the electron-phonon interaction and of the phonon density of states makes it possible to calculate the function $S(\omega)$. These calculations were made for a number of simple metals.[2] Calculation of $S(\omega)$ for transition metals and alloys is at present a practically unsolvable problem. In the absence of such calculation, McMillan's idea[3] of reconstructing the form of this function from experimental data on the tunnel characteristics of superconductor-normal metal junctions turned out to be very fruitful. By now, the form of the function $S(\omega)$ is known for very many metals and alloys.[4]

Knowing the function $S(\omega)$, the thermodynamic properties of the electrons of a normal metal can be calculated quite simply. In particular, the electron-phonon coupling constant λ, which determines the renormalization of the density of states of the electrons on the Fermi surface, and also the damping Γ of the excitations, are expressed in terms of this function in the following manner[5, 6]:

$$\lambda=2\int_0^\infty d\omega\frac{S(\omega)}{\omega},\quad \Gamma=2\pi\int_0^\infty d\omega S(\omega)[N(\omega)+f(\omega)]. \tag{1}$$

Here $N(\omega)$ and $f(\omega)$ are respectively the Bose and Fermi distribution functions:

$$N(\omega)=\frac{1}{e^{\omega/T}-1},\quad f(\omega)=\frac{1}{e^{\omega/T}+1}. \tag{2}$$

With the aid of the known Éliashberg equations,[7] the thermodynamic properties of the superconducting state are also expressed in terms of the function $S(\omega)$. Unfortunately, owing to the complexity of these equations, it is impossible to find their exact solution in the general case, so that it is impossible to write down in explicit form the functional dependence of the thermodynamic properties of superconductors on the function $S(\omega)$.

McMillan[8] was the first to obtain, as a result of an approximate solution of the Eliashberg equations, a formula for the critical temperature T_C of a superconductor, connecting this quantity with the function $S(\omega)$:

$$T_c=\frac{\Theta}{1.45}\exp\left[-\frac{1.04(1+\lambda)}{\lambda-\mu^+(1+0.62\lambda)}\right], \tag{3}$$

where Θ is the Debye temperature of this metal, μ^+ is the Coulomb pseudopotential:

$$\mu^+=\frac{\mu}{1+\mu\ln(\varepsilon_F/\Theta)}.$$

Dynes[9] has shown later that the critical temperatures are described much more accurately by the following expression, which no longer contains Θ, and all the quantities are expressed in terms of the function $S(\omega)$ only:

$$T_c=\frac{\langle\omega\rangle}{1.2}\exp\left[-\frac{1.04(1+\lambda)}{\lambda-\mu^+(1+0.62\lambda)}\right], \tag{4}$$

$$\langle\omega\rangle=\int_0^\infty d\omega S(\omega)\Big/\int_0^\infty d\omega\frac{S(\omega)}{\omega}. \tag{5}$$

Although the T_C calculated from both these formulas agree sufficiently well with their experimental values for many metals and alloys, many critical remarks were made concerning formulas (3) and (4).[10-12]

It became clear, above all, that these formulas describe poorly the critical temperatures for amorphous metals and alloys, where the functions $S(\omega)$ are quite large at low energies.[10] Moreover, arguments were advanced that these approximate formulas are not applicable at all to the description of the role of low-frequency phonons. In accordance with formulas (3)–(5), the softening of the phonon modes, i.e., the decrease of the phonon frequency, leads to an increase of T_C. These arguments are usually always cited as a confirmation of the idea that T_C increases in compounds such as A-15 and others, which are either unstable or are close to loss of stability.

Medvedev et al.[11] arrived, on the basis of an approximate solution of the Éliashberg equations, at the opposite conclusion, that T_c decreases or even vanishes when the frequency of at least one of the peaks in the phonon state density tends to zero. A similar statement is contained also in an earlier paper by Appel,[13] where it is stated that the presence of real thermal phonons with frequencies $\sim T_c$ leads to the damping of the Cooper pairs and to a decrease of T_c.

The second of the remarks concerning the McMillan formulas pertain to the possibility of determining the effectiveness of the contribution of various frequencies to the rise of T_c.[14, 15] We define this effectiveness in the following manner.

We introduce the change $\delta S(\omega)$ of the function

$$S(\omega)=S_0(\omega)+\delta S(\omega).$$

Then, in accordance with (4) and (5), the effectiveness $E(\omega)$ of the various frequencies is defined by

$$E(\omega)=\frac{\delta T_c}{\delta S(\omega)}=T_c\left[\frac{2}{\lambda\langle\omega\rangle}+\left(1.04\frac{1+0.38\mu^+}{[\lambda-\mu^+(1+0.62\lambda)]^2}-\frac{1}{\lambda}\right)\frac{2}{\omega}\right]. \quad (6)$$

The function $E(\omega)$ introduced in this manner, as seen from (6), depends essentially on the properties of the superconductor and behaves quite differently for superconductors with weak and strong coupling. Moreover, the physical situation arising when $E(\omega) \to \pm\infty$ as $\omega \to 0$ is clearly not physical.

On the other hand, the calculation of this function from the exact Éliashberg equations leads to entirely different results.[14] It turns out that $E(\omega)$ depends little on the concrete properties of the superconductor, and naturally $E(\omega) \to 0$ as $\omega \to 0$.

In this paper we attempt to look into the entire assembly of these problems in succession, and to establish the degree of reliability of the various approximate formulas for T_c. To this end we consider first the behavior of superconductors at $T \neq 0$ and establish certain characteristic properties that differ from those of superconductors at $T = 0$.

2. GENERAL PROPERTIES OF SUPERCONDUCTORS AT FINITE TEMPERATURES

To analyze the properties of superconductors, we use the well known Éliashberg equations[7, 1]

$$\Delta(\omega)Z(\omega)=\int_0^\infty d\omega'\,\mathrm{Re}\left\{\frac{\Delta(\omega')}{[\omega'^2-\Delta^2(\omega')]^{1/2}}\right\}\int_0^\infty d\omega_q S(\omega_q)\cdot$$
$$\cdot\{[f(-\omega')+N(\omega_q)]K_+(\omega',\omega_q,\omega)-[f(\omega')+N(\omega_q)]K_+(-\omega',\omega_q,\omega)\}$$
$$-\int_0^\infty d\omega'\,\mathrm{Re}\left\{\frac{\Delta(\omega')}{[\omega'^2-\Delta^2(\omega')]^{1/2}}\right\}[1-2f(\omega')]\mu(\omega',\omega), \quad (7)$$

$$[1-Z(\omega)]\omega=\int_0^\infty d\omega'\,\mathrm{Re}\left\{\frac{\omega'}{[\omega'^2-\Delta^2(\omega')]^{1/2}}\right\}\int_0^\infty d\omega_q S(\omega_q)\cdot$$
$$\cdot\{[f(-\omega')+N(\omega_q)]K_-(\omega',\omega_q,\omega)+[f(\omega')+N(\omega_q)]K_-(\omega',\omega_q,\omega)\}. \quad (8)$$

In these equations, $\mu(\omega',\omega)$ is the Coulomb interelectron repulsion, and in the simplest model that will be employed from now on we have

$$\mu(\omega',\omega)=\mu\Theta(\varepsilon_F-\omega')\Theta(\varepsilon_F-\omega),$$
$$K_\pm(\omega',\omega_q,\omega)=\frac{1}{\omega'+\omega_q+\omega+i\delta}\pm\frac{1}{\omega'+\omega_q-\omega-i\delta}. \quad (9)$$

The Éliashberg equations were solved many times numerically for $T = 0$, and the solutions of these equations for superconducting lead are shown schematically in Fig. 1. We see that $\mathrm{Im}\,\Delta(\omega) = 0$ for all frequencies $\omega < \Delta_0$ and $\mathrm{Re}\,\Delta(0) = \mathrm{const} \neq 0$.

This behavior of the ordering parameter at small ω leads to many well known characteristic features of the superconducting state. The excitation spectrum of the superconductor has an energy gap Δ_0, and in the density of states $N_S(\omega) = N(0)\,\mathrm{Re}\{\omega[\omega^2 - \Delta^2(\omega)]^{-1/2}\}$ there exists at $T = 0$ a forbidden energy region $\omega < \Delta_0$ in which $N_S(\omega) = 0$. In many studies of the properties of superconductors at $T \neq 0$, and unfortunately also in the calculation of T_c, it is assumed that the dependence of the ordering parameter on the frequency ω does not vary with temperature, and only the amplitude Δ changes, i.e.,

$$\Delta(\omega,T)=\Delta(\omega,T=0)\varphi(T).$$

The actual situation is quite different. It is easy to verify from Eq. (8) that at small ω we have

$$\mathrm{Re}\,Z(\omega)\approx 1+\lambda,\quad \mathrm{Im}\,Z(\omega)\approx\Gamma/\omega \quad (10)$$

where Γ is the damping of the electrons near the Fermi surface as the result of collisions with real thermal phonons:

$$\Gamma=2\pi\int_0^\infty d\omega\,N_s(\omega)S(\omega)[f(\omega)+N(\omega)]. \quad (11)$$

It is seen from (11) that at $T \geq T_c$, when $N_S = N(0)$, this formula goes over into Eq. (1) for the damping of electrons in a normal metal.

Using (7), we can show that as $\omega \to 0$ we have

$$\mathrm{Re}\,Z(\omega)\Delta(\omega)=\Sigma_1,\quad \mathrm{Im}\,Z(\omega)\Delta(\omega)=\omega\Sigma_2, \quad (12)$$

where Σ_1 and Σ_2 are certain constants, the exact solutions of which are immaterial at present. Further, it follows from (10)–(12) that at small ω we get

$$\mathrm{Re}\,\Delta(\omega)=\mathrm{Re}\frac{\Sigma_1+i\omega\Sigma_2}{Z(\omega)}\approx\omega^2\frac{\lambda\Sigma_1+\Gamma\Sigma_2}{\Gamma^2},$$
$$\mathrm{Im}\,\Delta(\omega)=\mathrm{Im}\frac{\Sigma_1+i\omega\Sigma_2}{Z(\omega)}\approx\omega\frac{\Sigma_1}{\Gamma}.$$

Consequently the state density of the electrons in the superconductor differs from zero at $T \neq 0$ for all ω, and in particular

$$N_s(0)=N(0)\Gamma/(\Sigma_1^2+\Gamma^2)^{1/2}.$$

In this respect, real superconductors, owing to the presence of inelastic scattering by real phonons and the ensuing damping processes, do not differ qualitatively in any way from superconductors with magnetic impurities, where there is also a finite density of state at all values of ω. There is, of course, a quantitative difference. In most real superconductors Γ is quite small. In particular, in the Debye model,

$$\Gamma\approx\lambda T(T/\Theta)^2. \quad (13)$$

S. Ginzburg[16] has already noted earlier that superconductors with nonmagnetic impurities having internal degrees of freedom, have at $T \neq 0$ a "gapless" state in analogy with superconductors with magnetic impurities.

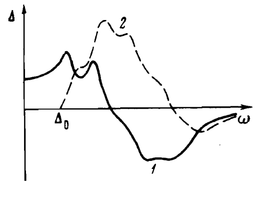

FIG. 1. Schematic form of the function $\Delta\omega$ for Pb at $T = 0$. Curve 1–$\mathrm{Re}\,\Delta(\omega)$, 2–$\mathrm{Im}\,\Delta(\omega)$.

The cause of this phenomenon lies precisely in the elastic scattering of the electrons with excitation of internal degrees of freedom of the impurity. We wish only to emphasize that for a "gapless" state to set in there is no need to introduce into the superconductors any impurities whatever. The role of these impurities in ordinary superconductors is played by the thermal phonons.

It is seen from (11) that a substantial difference between the behavior of real superconductors and their behavior in the BCS model arises only if vibrations with frequencies $\omega_q \sim T$ are present in the crystal. For most superconductors, as seen from (13), the effect of the thermal phonons is quite small. According to Appel's estimates,[13] it changes the thermodynamic properties of, say, lead, where the coupling constant is $\lambda = 1.3$, by not more than several per cent. These effects should come into play much more strongly in amorphous alloys and in compounds of the A-15 type, where owing to the proximity of the structural transformations or to the disordered character of the lattice there exists a rather appreciable softening of the phonon modes. In these situations, the problem of the effect exerted on the superconductivity by low-frequency phonons with $\omega_q \lesssim T_e$ becomes of major significance. The analogy with the magnetic impurities, which has already been mentioned in our paper, has led Appel[13] to an entirely incorrect conclusion that the thermal phonons, leading to damping in the ordering parameter Δ, lower T_c in the same way as the magnetic impurity. This problem will be considered in greater detail in Sec. 4 of the paper. But we note even now that thermal phonons differ greatly from magnetic impurities. Indeed, the presence of thermal phonons $N(\omega_q)$ leads to the onset of damping of the order parameter, but this very fact leads, in proportion to $N(\omega_q) + 1$, to the well known increase of the interelectron attraction due to the already existing boson excitations. This circumstance was not considered by Appel at all. As the excitation frequency $\omega_q \to 0$, these two effects cancel each other completely, so that oscillations with $\omega_q \ll T$, exert no direct influence on the thermodynamics of superconductors, in exactly the same manner as ordinary static impurities have no influence on the thermodynamics of superconductors.

In any case, however, allowance for the damping effect is essential when it comes to calculating the thermodynamic properties of superconductors accurate to T_c/Θ. It is also clear that the use of arbitrary variational functions for $\Delta(\omega)$ with $\operatorname{Re}\Delta(0) \neq 0$ to calculate the influence of the low-frequency phonons on T_c is absolutely illegitimate and leads to incorrect results.[10-12]

3. CRITICAL TEMPERATURE OF SUPERCONDUCTORS WITH WEAK AND INTERMEDIATE COUPLING

As already noted, in many real superconductors T_c is small in comparison with the characteristic phonon frequencies. Thus, even in lead, where $\lambda = 1.3$, the ratio is $T_c/\Theta \approx 0.1$. In this case we can neglect the influence of the thermal phonons and write down the Éliashberg equations, which determine T_c, in the form[7]

$$Z(\omega)\Delta(\omega) = \int_0^\infty \frac{d\omega'}{\omega'} \operatorname{Re}[\Delta(\omega')] \operatorname{th}\frac{\omega'}{2T_c} \cdot$$

$$\cdot \left[\int_0^\infty d\omega_q S(\omega_q) K_+(\omega', \omega_q, \omega) - \mu(\omega', \omega)\right],$$

$$\operatorname{Im} Z(\omega) = \frac{\pi}{\omega}\int_0^\omega d\omega_q S(\omega_q),$$

$$\operatorname{Re} Z(\omega) = 1 - \frac{1}{\omega}\int_0^\infty d\omega_q S(\omega_q) \int_{-\infty}^{+\infty} d\omega' f(-\omega') K_-(\omega', \omega_q, \omega). \qquad (14)$$

In these equations we have completely neglected the temperature effects wherever their order of magnitude is $(T_c/\bar{\omega})^2$, for example in $\operatorname{Im}Z(\omega)$, but have retained in part the temperature effects in $\operatorname{Re} Z(\omega)$, where they are of the order of smallness $(T_c/\bar{\omega})^2 \ln(\bar{\omega}/T_c)$[11, 12]. In particular, in the Debye approximation we have

$$\operatorname{Re} Z(0) = 1 + \Lambda(T_c) = 1 + \lambda\left[1 + \frac{2\pi^2}{3}\left(\frac{T_c}{\Theta}\right)^2 \ln\frac{\Theta}{T_c}\right]. \qquad (15)$$

The presence of such a temperature dependence of $\operatorname{Re} Z(0)$ can lead to a difference, say, between the ratio $2\Delta(0)/T_c$ and the universal value that follows from the BCS model.[12]

For convenience in the subsequent solution, we rewrite the first equation of (14) for Re in the form

$$\operatorname{Re}\Delta(\omega) = \varphi(\omega) = \int_0^\infty \frac{d\omega'}{\omega'} \varphi(\omega') \operatorname{th}\frac{\omega'}{2T_c}[L(\omega, \omega') - \tilde{\mu}(\omega, \omega')], \qquad (16)$$

where

$$L(\omega, \omega') = \operatorname{Re}\frac{1}{Z(\omega)}\int_0^\infty d\omega_q S(\omega_q) K_+(\omega', \omega_q, \omega),$$

$$\tilde{\mu}(\omega, \omega') = \operatorname{Re}\frac{1}{Z(\omega)}\mu(\omega, \omega'), \qquad L(0,0) = \frac{\lambda}{Z(0)}. \qquad (17)$$

Equation (16) has a logarithmic singularity in T_c and can be solved by the method developed in[17].

We make in (16) the substitution

$$\varphi(\omega')[L(\omega, \omega') - \tilde{\mu}(\omega, \omega')] = [L(\omega, 0) - \tilde{\mu}(\omega, 0)]\varphi(0)$$
$$+ \{[L(\omega, \omega') - \tilde{\mu}(\omega, \omega')]\varphi(\omega') - [L(\omega, 0) - \tilde{\mu}(\omega, 0)]\varphi(0)\}.$$

Then, introducing the function

$$\chi(\omega) = \frac{\varphi(\omega)}{\varphi(0)} \ln\frac{1.14\bar{\omega}}{T_c},$$

where $\bar{\omega}$ is as yet arbitrary frequency of the order of average phonon frequencies, we obtain

$$T_c = 1.14\bar{\omega} e^{-1/\chi(0)},$$

$$\chi(\omega) = [L(\omega, 0) - \tilde{\mu}(\omega, 0)] - A_{\omega'}\{[L(\omega, \omega') - \tilde{\mu}(\omega, \omega')]\chi(\omega')\}, \qquad (18)$$

where

$$A_\omega\{f(\omega)\} = \int_0^\infty d\omega \ln\frac{\omega}{\bar{\omega}} \frac{d}{d\omega} f(\omega).$$

The kernel of the integral equation (16) contains a short-range (in frequency) phonon part $L(\omega, \omega')$ and a long-range Coulomb part $\tilde{\mu}(\omega, \omega')$. We define accordingly also $\chi(\omega) = \chi_{ph}(\omega) + \chi_c(\omega)$, where $\chi_{ph}(\omega)$ is defined by

$$\chi_{ph}(\omega) = L(\omega, 0) - A_{\omega'}\{L(\omega, \omega')\chi_{ph}(\omega')\}. \qquad (19a)$$

It follows then for $\chi_c(\omega)$, from the preceding expression, that

$$\chi_c(\omega) = -\tilde{\mu}(\omega, 0)[1 - A_{\omega'}\{\chi_{ph}(\omega')\}] - A_{\omega'}\{[L(\omega, \omega') - \tilde{\mu}(\omega, \omega')]\chi_c(\omega')\}. \qquad (19b)$$

Introducing the notation

$$A_{\omega'}\{[L(0, \omega') - \tilde{\mu}(0, \omega')]\chi_c(\omega')\} = \mu(0, 0)\chi_c(0) \ln(\varepsilon_F/\bar{\bar{\omega}}),$$

we have

$$\chi_c(0) = -\frac{1}{Z(0)} \frac{\mu(0,0)[1 - A_{\omega'}\{\chi_{ph}(\omega')\}]}{1 + \mu(0,0)\ln(\varepsilon_F/\bar{\bar{\omega}})}.$$

It is easy to verify that $\bar{\bar{\omega}} \approx \bar{\omega}$ (i.e., of the order of the average phonon frequencies). A change of ω by even several times changes the Coulomb pseudopotential $\mu^+ = \mu/[1 + \mu\ln(\epsilon_F/\omega)]$ by not more than ten per cent, if it is recognized that $\epsilon_F \sim 1$ to 10 eV and $\bar{\omega} \sim 0.01$ eV.

In view of the crude character of the very model of the Coulomb interaction in the form of a certain constant μ up to $\omega = \epsilon_F$, and also in view of the inaccuracy with which μ^+ is determined from tunnel experiments, we shall not determine beforehand the exact value of $\bar{\bar{\omega}}$. We shall assume that

$$\chi_c(0) = -\frac{\mu^+}{Z(0)}[1 - A_{\omega'}\{\chi_{ph}(\omega')\}], \tag{20}$$

where μ^+ is a certain phenomenological constant.

Returning to the determination of χ_{ph} from (19b), we note that so far the quantity $\bar{\omega}$ has not been exactly defined. We can however redefine $\bar{\omega}$ in such a way as to make

$$A_{\omega'}\{L(0,\omega')\chi_{ph}(\omega')\} = 0. \tag{21}$$

Then

$$T_c = 1{,}14\bar{\omega}\exp\left\{-\frac{Z(0)}{\lambda - \mu^+(1+\alpha)}\right\}, \tag{22}$$

where

$$\alpha = -\int_0^\infty d\omega \ln\frac{\omega}{\bar{\omega}}\frac{d}{d\omega}\chi_{ph}(\omega), \tag{23}$$

$$\ln\bar{\omega} = -\frac{1}{L(0,0)\chi_{ph}(0)}\int_0^\infty d\omega \ln\omega \frac{d}{d\omega}[L(0,\omega)\chi_{ph}(\omega)], \tag{24}$$

and $\chi_{ph}(\omega)$ is defined by

$$\chi_{ph}(\omega) = L(\omega,0) + \int_0^\infty \frac{d\omega'}{\omega'}\left[L(\omega,\omega') - \frac{L(\omega,0)L(0,\omega')}{L(0,0)}\right]\chi_{ph}(\omega'). \tag{25}$$

Equation (25) can be solved by iteration, the small parameter in the iterations being $L(0,0) \approx \lambda/(1+\lambda)$. Since $L(0,0) < 1$ for all values of the coupling constant λ, the iteration series is certain to converge, but at $\lambda \gg 1$ it is entirely meaningless to solve Eq. (25), since all the temperature effects that are not small at $\lambda \gg 1$ have already been discarded in its very derivation.

Let us dwell briefly on our choice of $\bar{\omega}$ from the condition (21). This choice makes it possible to write down formally an expression for T_c in a form closest to the approximate McMillan formulas. Naturally, this choice of $\bar{\omega}$ is not unique. If another $\bar{\omega}$ is chosen, the exponential in the formula for T_c will differ already from that suggested by McMillan's formulas. This ambiguity in the choice of the pre-exponential factor and the exponential in the formula for T_c was already pointed out in[18, 19].

Kessel[19] solved the linearized Éliashberg equations by a method similar to that described in this paper. Owing to the somewhat different definition of the pre-exponential factor in the formula for T_c, the final expression obtained by Kessel contains in the argument of the exponential terms that are nonlinear in the coupling constant.

For the simplest model $S(\omega) = 1/2\lambda\omega_0\delta(\omega - \omega_0)$ an approximate formula containing in the argument of the exponential terms that are nonlinear in λ was obtained also by Hertel.[20] Our definition of the pre-exponential factor in the formula for T_c seems more natural, for in this definition $\bar{\omega}$ does not depend on the coupling constant λ, but only on the form of the spectral function $S(\omega)$.

As will be shown in the next section, sufficiently good agreement with exact T_c is obtained with the first iteration for $\chi_{ph}(\omega) = L(\omega, 0)$, which has already been used in (23) and (24). Moreover, as seen from (17) and $\operatorname{Re} Z(\omega)$ (14), the most significant change of $L(\omega, 0)$ as a function of ω is due to the change of the quantity

$$K_+(\omega,0) = \int_0^\infty d\omega_q S(\omega_q)\left(\frac{1}{\omega_q+\omega} + \frac{1}{\omega_q-\omega}\right).$$

We can therefore neglect the dependence of the function $Z(\omega)$ on the frequency, and put $Z(\omega) = 1 + \lambda$. We then obtain ultimately

$$\alpha = \frac{1}{1+\lambda}\int_0^\infty d\omega_q S(\omega_q)\ln\frac{\omega_q^2}{\bar{\omega}^2}, \tag{26}$$

$$\ln\bar{\omega} = \frac{2}{\lambda}\int_0^\infty \frac{d\omega_q}{\omega_q}S(\omega_q)\ln\omega_q$$

$$+\frac{2}{\lambda^2}\int_0^\infty \frac{d\omega_1}{\omega_1}S(\omega_1)\int_0^\infty d\omega_2 S(\omega_2)\ln\frac{\omega_1}{\omega_2}\left(\frac{1}{\omega_2+\omega_1} + \frac{1}{\omega_2-\omega_1}\right). \tag{27}$$

The expressions for α and $\bar{\omega}$ can be rewritten in a form that is more compact and more convenient for calculations

$$\bar{\omega} = \omega_{\text{лог}}e^{-A}, \quad \alpha = \lambda A/(1+\lambda),$$

$$\ln\omega_{\text{лог}} = \frac{2}{\lambda}\int_0^\infty \frac{d\omega_q}{\omega_q}S(\omega_q)\ln\omega_q,$$

$$A = -\frac{4}{\lambda^2}\int_0^\infty \frac{d\omega_1}{\omega_1}S(\omega_1)\ln\frac{\omega_1}{\omega_{\text{лог}}}K_+(\omega_1,0). \tag{28}$$

The table lists the results of calculations of T_c for a number of metals. The values of $S(\omega)$ were taken from the paper of Dynes, McMillan, and Rowell.[4] The same table lists for comparison the results of calculations of T_c using the approximate McMillan formulas, and also the results of Kessel's[19] iteration calculations of T_c. The agreement between the values of T_c calculated from (22) and (28) and the experimental data is quite good for all metals, with the possible exception of lead. For lead, where $\lambda = 1.3$, the use of the first iteration for $\chi(\omega)$ is not fully justified and it is therefore not surprising that the value of T_c also differs from the experimental one.

Let us consider briefly the expression for T_c in the case when $S(\omega)$ is represented by a sum of several δ functions. Let

$$S(\omega) = {}^1/_2\lambda_1\omega_1\delta(\omega-\omega_1) + {}^1/_2\lambda_2\omega_2\delta(\omega-\omega_2).$$

Then

$$\lambda = \lambda_1 + \lambda_2, \quad \omega_{\log} = \omega_1^{\lambda_1/\lambda}\omega_2^{\lambda_2/\lambda}, \tag{29}$$

and

$$A = \frac{1}{2} - \frac{\lambda_1\lambda_2}{2\lambda^2}\left[1 + \ln\frac{\omega_2}{\omega_1}\frac{\omega_1^2+\omega_2^2}{\omega_1^2-\omega_2^2}\right].$$

If the frequencies of two peaks do not differ very strongly from each other, i.e., if $\Delta\omega = |\omega_2 - \omega_1| \ll \omega_{1,2}$ then the second term in A is small like $(\Delta\omega/\omega)^2$ and can be neglected. In this case

$$T_c = \frac{\omega_{\log}}{1.43}\exp\left\{-\frac{1+\lambda}{\lambda - \mu^+[1+0.5\lambda/(1+\lambda)]}\right\}. \tag{30}$$

Comparing (30) with the McMillan formula (3), we see that these formulas practically coincide if $\omega_{\log}$ is identified with the Debye frequency of the superconduc-

Comparison of the calculated* values of T_c with the experimental T_c^{exp}

Metal	T_c^{exp}	$T_c^{(1)}$	$T_c^{(2)}$	$T_c^{(3)}$	$T_c^{(4)}$	A	Metal	T_c^{exp}	$T_c^{(1)}$	$T_c^{(2)}$	$T_c^{(3)}$	$T_c^{(4)}$	A
Pb	7.19	7.33	6.42	7.4	6,05	0.554	Hg	4,19	4,36	4,51		3.03	0.645
In	3.40	3.32	3,44		3.06	0.601	Tl	2.33	2.33	2.10		2.25	0.582
Sn	3.75	3.84	3.77	4.4	3.75	0.590	Ta	4.48	4.15	3.94		3.90	0.567

*$T_c^{(1)}$—calculated from the exact Eliashberg equation, $T_c^{(2)}$—from the approximate McMillan formulas, $T_c^{(3)}$—from the data of [19], $T_c^{(4)}$—from the approximate formulas (22) and (28). All the temperatures are in degrees Kelvin.

tor. This coincidence is not surprising if it is recalled that McMillan obtained his formula as a result of a numerical analysis of the dependence of T_c on the parameters of the spectrum of niobium. And, as is well known, the function $S(\omega)$ for niobium constitutes two narrow and close peaks. A formula that practically coincides with (30) was obtained for T_c also be Geĭlikman and Masharov.[21]

It must be emphasized that these formulas, as follows even from their derivation given in this paper, are valid only if $\omega_{1,2} \gg T_c$. But these formulas are known to be unsuitable for the description of the influence exerted on T_c by the low-frequency peaks with $\omega_q < T_c$. It is easy to verify with the aid of (29) and (30) that if the frequency of at least one of the peaks, say ω_1, tends to zero, and at the same time $\lambda_1 \neq 0$, then T_c also tends to zero. Actually this patently incorrect answer was indeed obtained in[11], where it is stated that the low-frequency phonons cause T_c to decrease. For a correct description of the low-frequency phonons in superconductors with strong coupling $\lambda > 1$, it is necessary to analyze the exact Éliashberg equations (7) and (8).

4. CRITICAL TEMPERATURE OF SUPERCONDUCTORS WITH STRONG COUPLING. ROLE OF LOW-FREQUENCY PHONONS

An exact analytic solution of Eqs. (7) and (8) in the presence of low-frequency phonons, with account taken of both the existence of thermal phonons and with the ensuing damping of the ordering parameter $\Delta(\omega)$ at $\omega = 0$, is practically impossible. Owing to the oscillatory dependence of $\Delta(\omega)$ on the frequency of phonons with small ω_q, the numerical solution of these equations leads to large errors. It is much more convenient to use in this case the Éliashberg equations in the temperature technique[21, 22]:

$$Z(i\omega_n)\Delta(i\omega_n)=\pi T_c \sum_{\omega_m=-\omega_{max}}^{\omega_{max}} [K(\omega_n-\omega_m)-\mu^+]\frac{\Delta(i\omega_m)}{|\omega_m|}, \tag{31}$$

$$[1-Z(i\omega_n)]\omega_n=-\pi T_c \sum_{\omega_m} \operatorname{sign}\omega_m K(\omega_n-\omega_m), \tag{32}$$

where

$$K(\omega_n-\omega_m)=2\int_0^\infty d\omega_q S(\omega_q)\frac{\omega_q}{\omega_q{}^2+(\omega_n-\omega_m)^2},$$
$$\omega_n=(2n+1)\pi T_c. \tag{33}$$

The summation in (31) is up to the maximum frequency $\omega_{max} \approx (5-10)\omega_D$. The limitation of the summation, as usual, is introduced to determine the Coulomb pseudopotential μ^+ in place of the direct Coulomb repulsion μ.

To calculate T_c it is necessary to solve the matrix equation (31). For superconductors with strong coupling, where $T_c \approx 0.1\omega_D$, the real rank of the matrix of this equation is quite small: $m_{max} \approx 5\omega_D/\pi T_c \approx 20$ and the time required to solve 20 such linear equations with a BÉSM-r computer is at worse several minutes.

The table contains the results of the calculation of T_c with the aid of Eqs. (31) and (32). The difference between the calculated and experimental values of T_c does not exceed several per cent and is apparently connected primarily with the inaccuracy in the determination of μ^+. We note that even for tantalum, where $\lambda = 0.69$, the rank of the matrix equation (31) is quite small, 63×63.

Before we proceed to calculate the dependences of T_c on the shapes and positions of the peaks in the phonon density of states, and to a comparison of the exact values of T_c obtained from the solution of (31) with the approximate formulas, we shall dwell briefly on the role of the low-frequency phonons with $\omega_q < T_c$.

Writing down $S(\omega) = S_1(\omega) + S_2(\omega)$, where the subscripts 1 and 2 pertain to oscillations with $\omega < T_c$ and $\omega > T_c$, respectively, we can write down in the same form also the kernel $K(\omega_n - \omega_m) = K_1(\omega_n - \omega_m) + K_2(\omega_n - \omega_m)$. As seen from (33), the only significant term in $K_1(\omega_n - \omega_m)$ is the one with $\omega_n = \omega_m$:

$$K_1(0)=\lambda_1=2\int_0^\infty d\omega_q \frac{S_1(\omega_q)}{\omega_q},$$

all the remaining terms are small like $\lambda_1(\omega_1/T_c)^2$. It is easy to verify with the aid of (32) that $Z(i\omega_n) = 1 + f_1(\omega_n) + f_2(\omega_n)$ where $f_1(\omega_n) = \lambda_1\pi T_c/|\omega_n|$. Substituting these expressions for K and Z in (31), we ultimately have

$$[1+f_2(i\omega_n)]\Delta(i\omega_n)+\frac{\pi T_c\lambda_1}{|\omega_n|}\Delta(i\omega_n)$$
$$=\frac{\pi T_c\lambda_1}{|\omega_n|}\Delta(i\omega_n)+\pi T_c\sum_{\omega_m}[K_2(\omega_n-\omega_m)-\mu^+]\Delta(i\omega_m). \tag{34}$$

We see therefore that all the terms with $S_1(\omega)$ in Eq. (34), which defines T_c, cancel out completely, and this cancellation is formally absolutely the same as in the case of static impurities.

The influence of phonon excitations that are supplementary to the already existing phonon spectrum and have different frequencies was considered in greater detail by Bergman and Rainer.[14] They have shown that phonon excitations with any frequency cause T_c to increase, but the measure of this increase $\delta T_c/\delta S(\omega) \to 0$ as the excitation frequency tends to zero. It was shown in their paper that the maximum contribution to T_c is made by the frequencies $\omega_q > 2\pi T_c$. Do the results obtained in this paper indicate that the softening of the phonon modes $\omega_q > 2\pi T_c$ always increases T_c? How accurately do the various approximate formulas describe this phenomenon? And what is the actual reason for the increase of T_c with decreasing frequency of the phonon oscillations? To answer these questions, we performed numerical experiments aimed at establishing the value of T_c for different spectral functions $S(\omega)$.

Since the available data on the spectra of real superconductors[4] are patently insufficient for a complete analysis of the problem, we used model spectra in the form of sums of two Lorentzians:

$$g_\nu(\omega)=A_\nu\left[\frac{1}{(\omega-\omega_1^{(\nu)})^2+(\omega_2^{(\nu)})^2}-\frac{1}{(\omega_2^{(\nu)})^2+(\omega_3^{(\nu)})^2}\right]$$

$$\text{if} \quad |\omega-\omega_1^{(\nu)}|<\omega_3^{(\nu)},$$

$$g_\nu(\omega)=0 \quad \text{if} \quad |\omega-\omega_1^{(\nu)}|>\omega_3^{(\nu)}.$$

The value of α_ν^2 was chosen by specifying the total electron-phonon coupling constant. By varying the position of one of the peaks, we calculated each time the

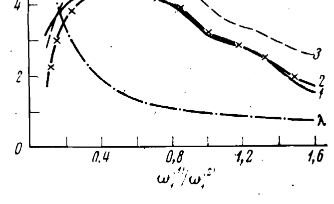

FIG. 2. Dependence of T_c on the relative position of the peaks in the model density of states: curve 1—"experimental" value of T_c, curve 2—T_c from formulas (22) and (28), curve 3—T_c from McMillan's formulas (4) and (5); $\lambda_0 = 0.7$; $\omega_1^{(2)} = 6$ meV.

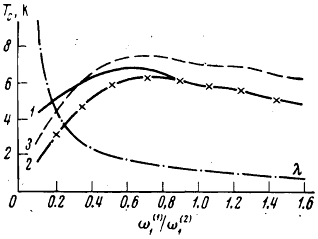

FIG. 3

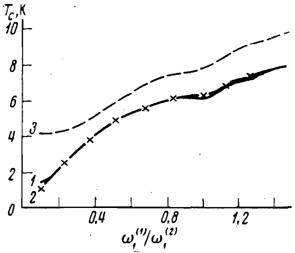

FIG. 4

FIG. 3. The same as in Fig. 2, but at $\lambda_0 = 1.0$ and $\omega_1^{(2)} = 6$ meV.

FIG. 4. The same as in Fig. 2, but at $\lambda = 1.0 = \text{const}$ and $\omega_1^{(2)} = 10$ meV.

value of T_c from the approximate McMillan formula (4), from the approximate formulas (22) and (28) of our paper, and from the exact solution of Eqs. (31) and (32). The last value of T_c can be conditionally called "experimental." The results of three runs of such calculations are shown in Figs. 2–4. The same figures show the values of the coupling constant λ as functions of the position of one of the peaks. In Figs. 2 and 3 the value of α_1^2 was not varied with changing $\omega_1^{(1)}$, and therefore the total coupling constant λ, defined by formula (1), increases with decreasing $\omega_1^{(1)}$. Figure 4 shows the result of the calculations of T_c with the total coupling constant invariant at $\lambda = 1$.

The diagrams show, first, that the two approximate formulas account qualitatively correctly for the behavior of the "experimental" T_c up to $\lambda \approx 2$, and the approximate formulas obtained in our paper are much more accurate than McMillan's formulas. The second result of these calculations is well noticeable when Figs. 2 and 3 with Fig. 4. The softening of the phonon frequencies (the decrease of $\omega_1^{(1')}$), if the total coupling constant is left unchanged (and all the more if it is decreased), leads only to a decrease of T_c. It follows therefore that to obtain an exact answer to the question of the feasibility of raising T_c in some compound by softening its phonon spectrum it is necessary to carry out a thorough analysis of the concomitant change of the electron-phonon coupling.

A third conclusion is precisely that practically the entire increase of T_c with decreasing $\omega_1^{(1)}$ is due only to the increase of λ, and the larger the initial $\lambda = \lambda_0$ the less the increase of T_c. The maximum value of T_c is reached at $\lambda \approx 2$, so that in Fig. 2, where $\lambda_0 = 0.7$, the peak in T_c is much less sharply pronounced than in Fig. 3, where λ_0 was set equal to unity. It is also clearly seen from these figures that in the presence of low frequencies $\omega_1 \approx T_c$ both approximate formulas give results that are certainly incorrect.

In Figs. 2 and 3 the value of T_c determined by the approximate formulas tends to zero as $\omega_1^{(1)} \to 0$. The finite width of the peak does not make it possible to perform a calculation with $\omega_1^{(1)} \ll T_c$ so as to be able to verify that the "experimental" T_c tends to a limit determined only by the second peak. Only in Fig. 4 can one note a deviation of the "experimental" value of T_c from the approximate that tends to zero, at the very smallest value of $\omega_1^{(1)}$.

Whether the existence of a small nonmonotonicity in T_c, in the case when the frequencies of two peaks coincide, is actually connected with the real dependence of T_c on the form of the function $S(\omega)$, or whether it is the result of an inaccuracy in the computer calculations, is a question that calls for further research.

In conclusion, we wish to express our sincere gratitude to many persons, discussions and talks with whom were quite useful to us–primarily to V. L. Ginzburg, D. A. Kirzhnits, Yu. V. Kopaev, Yu. M. Kagan, M. V. Medevedev, and many others.

---

[1] D. J. Scalapino, Superconductivity, 1, ed. R. D. Parks New York, 1969, p. 449.
[2] P. T. Truant, and J. P. Carbotte, Phys. Rev., B6, 3642 (1972).
[3] W. L. McMillan and J. M. Rowell, Superconductivity 1, ed. R. D. Parks, New York, 1969, p. 561.
[4] R. C. Dynes, W. L. McMillan and J. M. Rowell, Preprint Bell Lab., 1973.
[5] A. B. Migdal, Zh. Eksp. Teor. Fiz. **34**, 1438 (1958) [Sov. Phys.-JETP **7**, 996 (1958)].
[6] N. V. Zavaritskiĭ, Usp. Fiz. Nauk **108**, 241 (1972) [Sov. Phys.-Uspekhi **15**, 608 (1973)].
[7] G. M. Eliashberg, Zh. Eksp. Teor. Fiz. **39**, 1437 (1960) [Sov. Phys.-JETP **12**, 1000 (1961)].
[8] W. L. McMillan, Phys. Rev., **167**, 331 (1968).
[9] R. C. Dynes, Sol. St. Comm., **10**, 615 (1973).
[10] R. Benda, Phys. St. Sol., **38**, 451 (1969).
[11] M. V. Medvedev, E. A. Pashitskiĭ, and Yu. S. Pyatiletov, Zh. Eksp. Teor. Fiz. **65**, 1186 (1973) [Sov. Phys.-JETP **38**, 587 (1974)].
[12] C. R. Leavens and J. P. Carbotte, Can. J. Phys., **49**, 724 (1971).
[13] J. Appel, Phys. Rev. Lett., **21**, 1164 (1968).
[14] G. Bergman and D. Rainer, Zs. Phys., **263**, 59 (1973).
[15] C. R. Leavens, Sol. St. Comm., **14**, 37 (1974).
[16] S. L. Ginzburg, Zh. Eksp. Teor. Fiz. **59**, 478 (1970) [Sov. Phys.-JETP **32**, 262 (1971)].
[17] D. A. Kirznitz, E. G. Maximov and D. I. Khomskii, J. Low Temp. Phys., **10**, 791 (1973).
[18] M. V. Medvedev and Yu. S. Pyatiletov, Fiz. Met. Metalloved. **37**, 244 (1974).
[19] W. Kessel, Zs. Naturforsch., **29A**, 445 (1974).
[20] P. Hertel, Zs. Phys., **248**, 272 (1971).
[21] B. T. Geilikman and N. F. Masharov, J. Low Temp. Phys., **6**, 131 (1972).
[22] C. S. Owen and D. J. Scalapino, Physica, **55**, 691 (1971).

Translated by J. G. Adashko
208