ROLE OF THERMAL PHONONS IN HIGH-TEMPERATURE SUPERCONDUCTIVITY

J. Appel
John Jay Hopkins Laboratory for Pure and Applied Science,
Gulf General Atomic Incorporated, San Diego, California
(Received 16 May 1968)

With Éliashberg's equations for the two temperature Green's functions of a superconductor, the effect of real phonons on the transition temperature T_c is discussed. The equation derived for T_c/T_{c0} describes a temperature-dependent pair-breaking mechanism that depends on both the real and the imaginary part of the electron-phonon self-energy (T_{c0} = transition temperature in the absence of real phonons).

At finite temperatures, low-energy excitations such as acoustic phonons are thermally excited in a metal and interact with conduction electrons. In the normal state this interaction gives rise to a temperature dependence of the electrical resistivity. In the superconducting state this interaction, by virtue of its dynamical character, affects the energy gap and in particlar the transition temperature T_c. The electron-phonon (el-ph) interaction is usually described by Fröhlich's Hamiltonian which commutes with the time-reversal operator K for spin-$\frac{1}{2}$ particles. This Hamiltonian, however, depends on time-dependent phonon operators. Therefore, the theorem of Anderson[1] and Maki[2] does not apply, according to which T_c is unaffected by a perturbation that conserves time-reversal symmetry and is static. It is the purpose of this brief paper to study the effect of thermal phonons on T_c under the assumptions that (A) the mechanism for superconductivity, to begin with, consists in the exchange of virtual phonons between conduction electrons and (B) a mechanism other than the el-ph interaction causes superconductivity.

(A) The mathematical problem of determining T_c consists in solving the Éliashberg equations for the two Green's functions of a superconductor for temperatures $T \lesssim T_c$. Near T_c, the formal solutions of these equations are in the notation of Abrikosov, Gor'kov, and Dzyaloshinski[3] given by

$$\mathcal{G}(\epsilon,\vec{p}) = [i\epsilon - \xi(\vec{p}) + \Sigma_N(\epsilon,\vec{p};T)]^{-1} \tag{1}$$

$$\mathcal{F}^+(\epsilon,\vec{p}) = \mathcal{G}(\epsilon,\vec{p})\mathcal{G}(\epsilon,\vec{p})\Sigma_S(\epsilon,\vec{p};T), \tag{2}$$

where

$$\Sigma_N(\epsilon,\vec{p};T) = T(2\pi)^{-3}\sum_m \int d\vec{k}\,\mathcal{G}(\omega,\vec{k})\,\mathfrak{D}(\epsilon-\omega;\vec{p}-\vec{k}), \tag{3}$$

$$\Sigma_S(\epsilon,\vec{p};T) = T(2\pi)^{-3}\sum_m \int d\vec{k}\,\mathcal{F}^+(\omega,\vec{k})\,\mathfrak{D}(\epsilon-\omega;\vec{p}-\vec{k}). \tag{4}$$

Here $\omega = (2m+1)\pi T$. The el-ph coupling constant g^2 is contained in the phonon Green's function $\mathfrak{D}$. The electron Green's function $\mathcal{G}$ in the normal state depends on T through the variable $\epsilon = (2n+1)\pi T$ and through the T dependence of the self-energy Σ_N. The latter is due to the change of electron and phonon occupation numbers with T. Because of the T dependence of Σ_N, the pairing energy in the superconducting state Σ_S has an additional temperature dependence, beyond that which is of the BCS form.

To solve the linear integral Eq. (4), after eliminating the momentum dependence of Σ_S with a quadrature,[4-7] Swihart, Scalapino, and Wada[6] and Wu[8] have applied an interation method. Their result for T_c contains the effect of thermal phonons. The transition temperature in the absence of thermal phonons T_{c0} is not evaluated by these authors. To find T_{c0}, one must replace $\Sigma_N(\epsilon,\vec{p};T)$ in Eqs. (3) and (4) with $\Sigma_N(\epsilon,\vec{p};0)$, where $\Sigma_N(\epsilon,\vec{p};0)$ is the self-energy in the limit $T=0$ (see Ref. 7, p. 200). Whether this numerical calculation has been carried out is not known to us.

In this Letter a simple analytical expression is derived for T_c/T_{c0} which accounts for the temperature dependence of the real and imaginary part of Σ_N.[9] The analytic continuation of the self-energy has been calculated by AGD[3] and the result can be written in the form

$$\mathrm{Re}\Sigma_N(\epsilon,p_F;T) = [m - m^*(T)]m^{-1}\epsilon, \tag{5}$$

$$\mathrm{Im}\Sigma_N(\epsilon,p_F;T) = (\mathrm{sgn}\epsilon)/2\tau(\epsilon,p_F;T), \tag{6}$$

where

$$\frac{m-m^*(T)}{m}=\frac{g^2}{16\pi^2}\frac{m}{p_F}\int_0^{2p_F}qdq\,\omega^2(q)\mathrm{P}\int_{-\infty}^{+\infty}\frac{1-\tanh^2x}{(2Tx)^2-\omega^2(q)}dx, \tag{7}$$

$$\frac{1}{\tau(\epsilon,p_F;T)}=\frac{g^2}{4\pi}\frac{m}{p_F}\int_0^{2p_F}qdq\,\omega(q)\frac{e^{\epsilon/T}+1}{e^{\omega(q)/T}-1}\left(\frac{1}{e^{\epsilon/T}+e^{-\omega(q)/T}}+\frac{1}{e^{[\epsilon-\omega(q)]/T}+1}\right). \tag{8}$$

The el-ph scattering time given by the last equation is exactly equal to the cyclotron-resonance relaxation time in the theory of Azbel' and Kaner.[10] Equations (5)-(8) give the self-energy for electrons in the vicinity of the Fermi surface. In this approximation the retarded Green's function is given by[11]

$$G_R=a/[\epsilon-\Xi(\vec{p})+ia/2\tau], \tag{9}$$

where $\Xi=a\xi$ and $a=m/m^*(T)$. From the retarded Green's function G_R, one finds the thermodynamic Green's function $\mathcal{G}$ in the manner described by AGD.[3] If one inserts this $\mathcal{G}$ into the equation for $\mathfrak{F}^+$, the energy-gap equation near T_c becomes

$$\Sigma_S(\epsilon,\vec{p};T)=\frac{T}{(2\pi)^3}\sum_m\int d\vec{k}\,\mathfrak{D}(\epsilon-\omega;\vec{p}-\vec{k})\frac{a^2\Sigma_S(\omega,\vec{k};T)}{\omega^2\eta^2+\Xi^2(\vec{k})}, \tag{10}$$

where $\eta=1+a/2\tau(T)|\omega|$. $\tau(T)$ is given by Eq. (8). To solve this equation, we make the BCS approximation and take $\mathfrak{D}=-g^2$. Correspondingly, Σ_S becomes a constant and Eq. (10) becomes the defining equation for T_c. It is of the same form as the T_c equation derived by Gor'kov and Abrikosov[12] in studying the effect of paramagnetic impurities on superconductivity.

The solution for T_c is of a simple form in the special (though unreal) case where $T_{c0}\gg\Theta_D$ (=Debye temperature). The point is that at temperatures $T\gg\Theta_D$, the real part of the self-energy becomes small, $m^*(T)\to m$. If one ignores $\mathrm{Re}\Sigma_N$, the result for T_c is given by

$$\ln\left(\frac{T_{c0}}{T_c}\right)=\psi(\tfrac{1}{2}+x)-\psi(\tfrac{1}{2})\quad(T_{c0}\gg\Theta_D), \tag{11}$$

where $\psi(x)$ is the di-gamma function and $x=\frac{1}{4}\pi T_c\tau(T_c)$. The transition temperature in the absence of thermal phonons is given by the BCS-Gor'kov formula $T_{c0}=1.14\Theta_D\exp[-1/(\lambda-\mu^*)]$, where $\lambda=N(0)g^2$ and μ^* are the el-ph and Coulomb coupling constants, respectively; $N(0)=mp_F/2\pi^2$.

In real superconductors $T_c<0.1\Theta_D$ and, therefore, the real part of the self-energy must be taken into account. Its temperature dependence is according to Eq. (5) determined by $m^*(T)$ (see Fig. 1). If one includes $\mathrm{Re}\Sigma_N$, the equation for T_c becomes

$$\ln\left(\frac{T_{c0}}{T_c}\right)+\left\{\frac{1}{[N(0)V]_{\mathrm{BCS}}{}^0}-\frac{1}{[N(0)V]_{\mathrm{BCS}}{}^{T_c}}\right\}=\psi(\tfrac{1}{2}+y)-\psi(\tfrac{1}{2})\quad\text{(general case)}, \tag{12}$$

where $[N(0)V]_{\mathrm{BCS}}{}^T=a(T)\lambda-\mu^*$ and $y=a/4\pi T_c\tau$. In the absence of thermal phonons, the transition temperature $T_{c0}=1.14\Theta_D\exp\{-1/[N(0)V]_{\mathrm{BCS}}{}^0\}$. This formula for T_{c0} is similar to that found by McMillan[9] for strongly coupled superconductors. The solution of Eq. (12) is plotted in Fig. 2 as curve A, using the approximation $\psi(\frac{1}{2}+y)-\psi(\frac{1}{2})=\frac{1}{2}\pi^2y$. To summarize, the effect of thermal photons on T_c is at most of the order of 20% corresponding to the unreal case where $T_{c0}/\Theta_D\simeq0.3$. In real and strongly coupled superconductors the effect is a few percent. As examples let us consider Pb and Nb_3Sn.

According to Eq. (12), T_c depends on four parameters: λ, μ^*, $a(T)$, and $\tau(T)$. For lead we take $\lambda=1.3$ and $\mu^*=0.1$.[9] The function $a(T)=m/m^*(T)$ is determined from Fig. 1. The scattering time $\tau(T)$

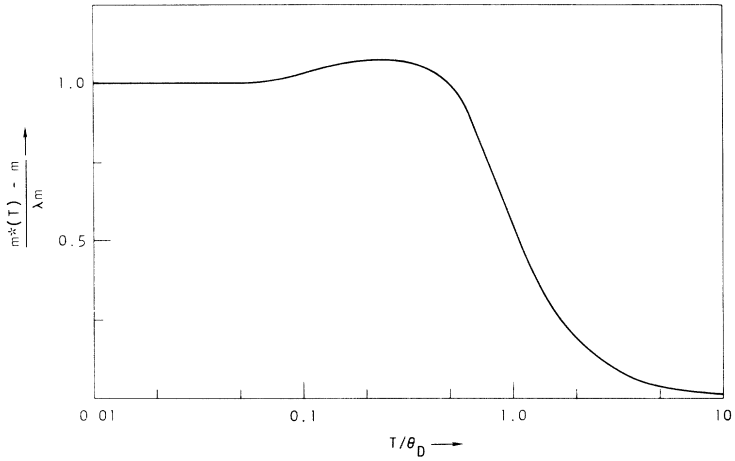

FIG. 1. Temperature dependence of the renormalized electron mass $m^*(T)$ defined by using Eq. (5) for the real part of the el-ph self energy.

is found from the equation

$$\tau(T) = 17.3(T/\Theta_D)^2 \tau_{tr}(T), \quad T \ll \theta. \tag{13}$$

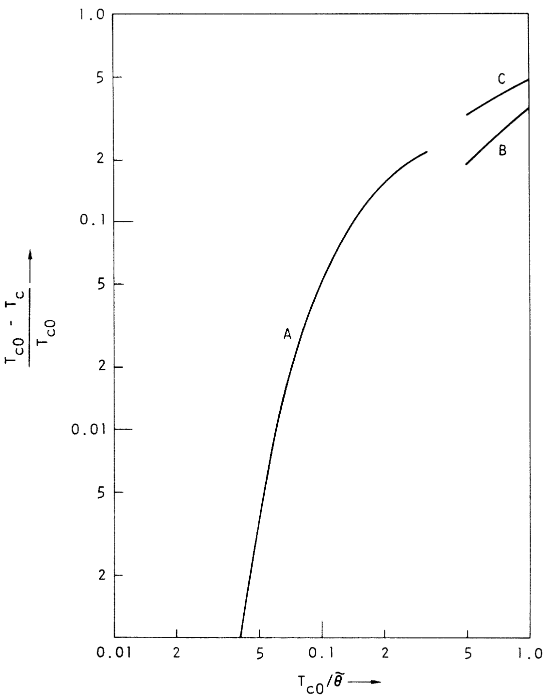

FIG. 2. Effect of thermal phonons on the transition temperature. Curve A (phonon mechanism) presents the solution of Eq. (12) $\tilde{\theta} = \Theta_D$. Curves B and C (nonphonon mechanism) present the solutions of Eq. (17) for $\tilde{\theta}/\Theta_D = 1$ and $\tilde{\theta}/\Theta_D = 2$, respectively; the el-el interaction is attractive in a shell of thickness $2\tilde{\theta}$ around the Fermi surface. The interaction between electrons and thermal phonons is in both cases B and C characterized by the el-ph coupling parameter $\lambda = 1$.

Here the transport time τ_{tr} is determined by the electrical resistivity $\rho = \frac{2}{3}e^2\tau_{tr}N(0)v_F^2$ where $v_F = p_F/m$. From Van den Berg's resistivity measurements on lead[13] one finds $\tau(T_c = 7.2°K) = 1.15 \times 10^{-11}$ sec, in good agreement with the theoretical value of 1.8×10^{-11} sec that follows from Eq. (8) with $\lambda = 1.3$. With the experimental value of $\tau(T_c)$, one finds the result that $(T_{c0} - T_c)/T_{c0} = 0.031$.

On the other hand, for Nb_3Sn the pertinent parameter $a(T_c)\pi/8T_c\tau(T_c)$ has the unrealistic value of ~2 if one assumes that $\tau_1 = \tau_{sd}$. The scattering time τ_{sd} is found from the experimental resistivity values of Cohen, Cody, and Halloran[14] using the relation $\rho_{sd} = \frac{2}{3}e^2\tau_{sd}N_s(0)v_{Fs}^2$; $N_s(0)$ is the density of states at the s part of the Fermi surface and is by a factor 50 smaller than density of states at the d part; $v_{Fs} = 10^8$ cm/sec. It is obvious that our assumption $\tau_1 = \tau_{sd}$ is wrong if the d electrons govern superconductivity,[15] and not the s electrons which carry the electric current in the normal state.

(B) To discuss the effect of thermal phonons on T_c when not the el-ph interaction but a mechanism of the type proposed by Matthias[16] for transition metals (d-shell polarization) leads to superconductivity, let us presume a Hamiltonian of the BCS-Gor'kov form.[3] The el-el interaction is attractive in a shell $2\tilde{\omega}$ around the Fermi surface and the coupling parameter is κ^2. The energy gap equation near T_c is given by

$$\Delta = \kappa^2 T(2\pi)^{-3}\sum_m \int d\vec{k}\, \mathfrak{F}^+(\omega, \vec{k}), \tag{14}$$

where

$$\mathfrak{F}^+(\omega, k) = \mathcal{G}(\omega, \vec{k})\mathcal{G}(-\omega, \vec{k})[\Delta + \bar{\mathfrak{F}}^+(\omega, \vec{k})], \tag{15}$$

with $\mathcal{G}$ given by Eq. (1). Let us assume that $\overline{g^2} \ll \kappa^2$. Then, at the Fermi surface one has

$$\bar{\mathfrak{F}}^+/\Delta = \lambda \ln(1.14\Theta_D/T_c). \tag{16}$$

With Eq. (15), the defining equation for T_c is found from Eq. (14) in the form

$$\ln\left(\frac{T_{c0}}{T_c}\right) + \frac{a(T_c)-a(0)}{a(T_c)a(0)} \frac{1}{\kappa^2 N(0)[1+\lambda \ln(1.14\Theta_D/T_c)]} = \psi(\tfrac{1}{2}+y) - \psi(\tfrac{1}{2}), \tag{17}$$

where a and y are the same parameters as in Eq. (12) and where

$$T_{c0} = 1.14\tilde{\theta} \exp\{-1/\kappa^2 N(0)[1+\lambda \ln(1.14\Theta_D/T_c)]\}.$$

For two cases, $\tilde{\omega}/\omega_D = 1$ (curve A) and $\tilde{\omega}/\omega_D = 2$ (curve B), the solutions for T_c/T_{c0} are plotted in Fig. 2. A realistic value is chosen for the el-ph coupling constant, namely $\lambda = 1$. It is seen that the interaction between electrons and thermal phonons does not preclude the occurrence of room-temperature superconductivity but can reduce T_{c0} by a factor 2 if $T_{c0} \sim \tilde{\theta}$.

It is a pleasure to thank Professor W. Kohn for constructive discussions. I am indebted to Dr. T. W. Mihalisin, Dr. L. W. Nordheim, Dr. B. W. Roos, and Professor D. J. Scalapino for helpful comments.

[1]P. W. Anderson, J. Phys. Chem. Solids 11, 26 (1959).

[2]K. Maki, in "A Treatise on Superconductivity," edited by R. D. Parks (Marcel Dekker, New York, to be published).

[3]A. A. Abrikosov, L. P. Gor'kov, and I. E. Dzyaloshinski, in Methods of Quantum Field Theory in Statisical Mechanics, edited by R. Silverman (Prentice-Hall Inc., Englewood Cliffs, N.J., 1963), p.280; referred to as AGD.

[4]V. Ambegoakar and L. Tewordt, Phys. Rev. 134, A805 (1965).

[5]V. Wada, Phys. Rev. 135, A1481 (1964).

[6]J. C. Swihart, D. J. Scalapino, and J. Wada, Phys. Rev. Letters 14, 106 (1965).

[7]J. R. Schrieffer, Theory of Superconductivity (W. A. Benjamin, Inc., New York, 1964), p. 193.

[8]T. M. Wu, Phys. Rev. Letters 19, 508 (1967).

[9]W. L. McMillan, Phys. Rev. 167, 331 (1968), discusses the importance of the real part of the self-energy (at $T=0$ and $\epsilon=0$) in calculating T_{c0} for strongly coupled superconductors.

[10]M. Ya. Azbel' and E. A. Kaner, J. Phys. Chem. Solids 6, 113 (1958).

[11]S. Nakajima and M. Watabe, Progr. Theoret. Phys. (Kyoto) 29, 341 (1963). Equation (9) is based on the expression (5) for the real part of Σ_N. This approximation for $\mathrm{Re}\Sigma_N$ is equivalent with taking the renormalization factor $Z(\epsilon)$ at the Fermi surface, $\epsilon=0$ (see Ref. 6).

[12]A. A. Abrikosov and L. P. Gor'kov, Zh. Eksperim. i Teor. Fiz. 39, 1781 (1961) [translation: Soviet Phys. –JETP 12, 1243 (1961)].

[13]G. J. Van den Berg, Physica 14, 111 (1948).

[14]R. W. Cohen, G. D. Cody, and J. J. Halloran, Phys. Rev. Letters 19, 840 (1967).

[15]C. G. Shull and F. A. Wedgwood, Phys. Rev. Letters 16, 513 (1966); see also G. Gladstone, M. A. Jensen, and J. R. Schrieffer, in "A Treatise on Superconductivity," edited by R. Parks (Marcel Dekker, New York, to be published).

[16]P. W. Anderson and B. Matthias, Science 144, 373 (1964). For a discussion of mechanisms leading to superconductivity in transition metal alloys, see also T. H. Geballe, Rev. Mod. Phys. 36, 134 (1964); B. R. Coles, Rev. Mod. Phys. 36, 139 (1964).