Some effects of phonon dynamics on electron lifetime, mass renormalization, and superconducting transition temperature*

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Effects of the dynamical properties of phonons on the electronic properties of metals are treated through the use of the phonon spectral weight function. It is shown that the leading behavior of the electron quasiparticle lifetime is lowered to quadratic in the frequency or temperature from the cubic behavior which is well known to occur for infinitely sharp phonons. Explicit evaluations of $1/\tau$ are made using an extension of the Debye model which allows for a finite phonon lifetime. The mass-enhancement parameter λ is discussed and is shown formally to be related to the static phonon propagator. Thus if there is a difference between the phonon relaxation at zero frequency and at the phonon frequency, it is possible for the phonon frequencies which determine λ to differ significantly from the peak frequencies observed in inelastic neutron scattering. The implications of these results for superconducting transition temperatures are discussed with particular reference to recent neutron scattering experiments in Nb_3Sn.

I. INTRODUCTION

The influence of electron-phonon interactions on the properties of electrons near the Fermi surface of metals has been the subject of much recent activity.[1] Progress in tunneling spectroscopy[2] has made possible detailed measurements of the electron-phonon spectral function $\alpha^2F(\omega)$, from which one can deduce the effects of phonons on the electronic properties. Field-theoretic techniques has been used to demonstrate that lowest-order theories are accurate to order $(m/M)^{1/2}$, where m and M are the electron and ion mass, respectively.[3]

It is well known that the phonon system itself has a complicated dynamics and a potential richness of structure far beyond the capabilities of harmonic Born-von Karman–type theories to describe. Field-theoretic techniques have been developed[4] to aid in the description of phonon dynamics when complications such as anharmonic effects, disorder or impurity effects, electron-phonon interactions, or structural instability are present. However, it has usually been considered adequate to treat the phonons as infinitely sharp excitations when studying their role in modifying electronic properties. In this paper, we will utilize the field-theoretic techniques to include the complete phonon dynamics in the study of the behavior of electrons near the Fermi surface. We will demonstrate, in particular, that the leading behavior in temperature and frequency is modified from the infinite-lifetime phonon result.

The organization of this paper is as follows. In Sec. II we describe the phonon spectral weight function $B(\vec{Q}, \omega)$ which contains all the necessary information on phonon dynamics. We show that the phonon density of states $F(\omega)$, as defined rigorously in terms of $B(\vec{Q}, \omega)$, scales as ω instead of ω^2 as the frequency ω goes to zero. We then incorporate the function $B(\vec{Q}, \omega)$ into our calculations of electronic properties. In Sec. III we discuss the quasiparticle lifetime τ for electrons near the Fermi surface, and in particular the leading behavior of $1/\tau$ in temperature (T) and frequency (ω). We find that instead of the usual T^3 or ω^3 behavior expected for $1/\tau$ from electron-phonon scattering, the inclusion of dynamical processes in the phonon spectral function alters the leading behavior to T^2 or ω^2. In Sec. IV, the particular case of electron-phonon-limited phonon lifetimes is discussed. In Sec. V, an extension of the Debye model is made to allow the inclusion of finite phonon lifetimes. Detailed calculations are made for $\alpha^2F(\omega)$ and $1/\tau(T, \omega)$ in this model. In Sec. VI, the electron mass-enhancement parameter λ is discussed.

II. PHONON SPECTRAL WEIGHT FUNCTION

The phonon spectral weight function $B(\vec{Q}, \omega)$ is defined as (e.g., Scalapino in Ref. 1)

$$D(\vec{Q}, i\omega_\nu) = \int_{-\infty}^{\infty} d\omega B(\vec{Q}, \omega)(i\omega_\nu - \omega)^{-1} , \qquad (1)$$

where $D(\vec{Q}, i\omega_\nu)$ is the Green's function for phonons at wave vector $\vec{Q}$ and imaginary frequency $i\omega_\nu = 2\pi i\nu/\beta\hbar$, and β is the inverse temperature $(k_B T)^{-1}$. In what follows, we will typically set $\hbar$ equal to

1, except for final formulas, where $\hbar$ will be restored. The physical interpretation of the spectral weight function is that a single lattice wave of wave vector $\vec{Q}$ is not an eigenstate of the crystal if interactions (such as anharmonic or electron phonon) are present. The lattice wave is a superposition of exact eigenstates with a quasicontinuous distribution of energies rather than a fixed energy. The function $B(\vec{Q}, \omega)$ describes this distribution of energy.

Using the definition of the phonon Green's function,[1] the following expression can be derived for $B(\vec{Q}, \omega)$ in terms of the exact crystal eigenstates $|n\rangle$ and energies E_n:

$$B(\vec{Q}, \omega) = \sum_{m,n} (e^{-\beta E_n} - e^{-\beta E_m}) |\langle m| \varphi^*_{\vec{Q}} |n\rangle|^2 \times \delta(\omega - E_m + E_n) \Big/ \sum_n e^{-\beta E_n} . \quad (2)$$

From Eq. (2) one sees immediately that $B(\vec{Q}, \omega)$ is an odd function of ω. In general, one expects $B(\vec{Q}, \omega)$ to vary linearly with ω at small ω. For noninteracting phonons, however, the linear term vanishes, and $B(\vec{Q}, \omega)$ becomes

$$B_0(\vec{Q}, \omega) = \delta(\omega - \omega_{\vec{Q}}) - \delta(\omega + \omega_{\vec{Q}}) , \quad (3)$$

where $\omega_{\vec{Q}}$ is the phonon frequency and the subscript zero indicates noninteracting. The phonon density of states can be defined as

$$F(\omega) = \sum_{\vec{Q}} B(\vec{Q}, \omega) \quad (\omega > 0) . \quad (4)$$

For noninteracting phonons, this becomes

$$F_0(\omega) = \sum_{\vec{Q}} \delta(\omega - \omega_{\vec{Q}}) . \quad (5)$$

The leading behavior (at small ω) is ω^2 (from phase-space arguments, assuming an acoustic spectrum). There are sharp Van Hove singularities coming from regions of phase space where $|\nabla_{\vec{Q}} \omega_{\vec{Q}}|$ vanishes. In general, B is linear in ω, and thus the leading behavior of F is also linear for the interacting case, Eq. (4). Also, the Van Hove singularities will, in general, be smeared out.

We can now incorporate the phonon spectral function into calculations of the electronic properties. According to Migdal's arguments,[3] low-order perturbation theory gives a highly accurate formula for the self-energy $\Sigma(\vec{k}, \omega)$ of an electron of wave vector $\vec{k}$ arising from electron-phonon interactions. The resulting formula for Σ can be written

$$\Sigma(\vec{k}, \omega - i\delta) = \Sigma_1(\vec{k}, \omega) + i\Sigma_2(\vec{k}, \omega) = \int_{-\infty}^{\infty} d\omega' \int_0^{\infty} d\Omega\, \alpha^2 F(\vec{k}, \Omega) \times \left(\frac{f(\omega') + N(\Omega)}{\omega - \omega' + \Omega - i\delta} + \frac{1 - f(\omega') + N(\Omega)}{\omega - \omega' - \Omega - i\delta} \right) . \quad (6)$$

In this formula, f and N are the Fermi and Bose function, respectively. The information about the phonons and the electron-phonon coupling is all contained in the electron-phonon spectral function $\alpha^2 F(\vec{k}, \omega)$ which can be rigorously defined (Scalapino, Ref. 1) in terms of the phonon spectral function $B(\vec{Q}, \omega)$:

$$\alpha^2 F(\vec{k}, \omega) = \sum_{\vec{Q}} |M(\vec{k} - \vec{k} + \vec{Q})|^2 B(\vec{Q}, \omega) \delta(\epsilon_{\vec{k}+\vec{Q}}) , \quad (7)$$

$$\alpha^2 F(\omega) = \sum_{\vec{k}} \alpha^2 F(\vec{k}, \omega) \delta(\epsilon_{\vec{k}}) \Big/ \sum_{\vec{k}} \delta(\epsilon_{\vec{k}}) . \quad (8)$$

In Eq. (7), M is the matrix element for an electron-phonon scattering to occur between electron states $\vec{k}$ and $\vec{k} + \vec{Q}$. The final electron state $\vec{k} + \vec{Q}$ is compelled to lie on the Fermi surface and the initial state is fixed. The average of $\alpha^2 F(\vec{k}, \omega)$ over the Fermi surface gives $\alpha^2 F(\omega)$ [Eq. (8)] which is the function measured in tunneling experiments.[2]

If $B(\vec{Q}, \omega)$ is approximated by a δ function, then $\alpha^2 F(k, \omega)$ and $\alpha^2 F(\omega)$ are both quadratic in ω at small ω, as is the density of states $F(\omega)$ as given in Eq. (5). This happens because the matrix element M^2 contributes a factor Q while the factor $\delta(\epsilon_{\vec{k}+\vec{Q}})$ contributes a canceling factor, Q^{-1}. Experimentally, it has been observed[5] that $\alpha^2 F(\omega)$ is remarkably similar to $F(\omega)$ in materials like Pb. The introduction of phonon dynamics through the spectral function B can be expected to convert the low-frequency behavior of $\alpha^2 F$ from quadratic to linear in ω [in precisely the same way as occurs for the density of states $F(\omega)$]. In fact, in amorphous metals, where the lattice wave vector is no longer a conserved quantity and consequently the phonon damping is large, the linear region in $\alpha^2 F(\omega)$ has been observed.[6] The consequences of the linear behavior of $\alpha^2 F$ for electronic properties will be discussed in Secs. II–IV.

III. ELECTRON LIFETIME

The quasiparticle lifetime of an electron due to electron-phonon scattering is given by the imaginary part of the self-energy of Eq. (6):

$$\frac{1}{2\tau(\vec{k}, \epsilon)} = -\Sigma_2(\vec{k}, \epsilon) = \pi \int_0^{\infty} d\Omega\, \alpha^2 F(\vec{k}, \Omega) \times [2N(\Omega) + f(\Omega + \epsilon) + f(\Omega - \epsilon)] . \quad (9)$$

Measurable electron lifetimes are not given directly by Eq. (9), but rather by some average of Eq. (9). This average is taken over a portion of Fermi surface (such as an external orbit in Azbel-Kaner resonance), and also over an effective thickness in energy ϵ. We shall not concern ourselves with the Fermi-surface average (which varies with the experiment), but the energy average has a simple form, which can be deduced

from rigorous transport theories such as that of Scher and Holstein.[7] Thus,

$$1/\tau(\vec{k}, \omega, T) = \int (d\epsilon/2\omega)[f(\epsilon) - f(\epsilon+\omega)] \times [1/\tau(\vec{k}, \epsilon) + 1/\tau(\vec{k}, \epsilon+\omega)] . \quad (10)$$

When ω is very small ($\hbar\omega \ll k_B T$, $\hbar\omega_D$) this averaging process acquires a form familiar from the semiclassical Boltzmann equation[8]

$$\frac{1}{\tau(\vec{k}, T)} = \int d\epsilon \left(-\frac{\partial f}{\partial \epsilon}\right) \frac{1}{\tau(\vec{k}, \epsilon)} . \quad (11)$$

Inserting the formula for $1/\tau$ from Eq. (9), we can integrate Eq. (11) yielding[9]

$$1/\tau(\vec{k}, T) = 4\pi\hbar(k_B T)^{-1} \int_0^\infty d\Omega\, \Omega \alpha^2 F(\vec{k}, \Omega) N(\Omega) \times [N(\Omega)+1] \quad (\hbar\omega \ll k_B T;\ \omega \ll \omega_D) . \quad (12)$$

Another easily treated limiting case is that of low temperature, $k_B T \ll (\hbar\omega, \hbar\omega_D)$. In this limit Eq. (9) and (10) can be simplified to yield[10]

$$1/\tau(\vec{k}, \omega) = 2\pi\omega^{-1} \int_0^\omega d\Omega(\omega - \Omega)\alpha^2 F(\vec{k}, \Omega) \quad (k_B T \ll \hbar\omega, \hbar\omega_D) . \quad (13)$$

It is now easy to show from Eqs. (12) and (13) that the limiting behavior of $1/\tau$ at low T and ω is T^{n+1} and ω^{n+1} provided that function $\alpha^2 F$ scales as Ω^n for small Ω. Thus $1/\tau$ scales as T^3 and ω^3 for infinitely sharp phonons, but as T^2 and ω^2 when the linear term in $B(\vec{Q}, \omega)$ is finite. More specifically, the quadratic terms are given by

$$1/\tau(\vec{k}, \omega, T) = (\pi/3\hbar^2) D_{\vec{k}} [(2\pi k_B T)^2 + (\hbar\omega)^2] . \quad (14)$$

This equation is valid for very small T and ω. The coefficient $D_{\vec{k}}$ is defined by

$$D_{\vec{k}} = \frac{d}{d\omega}[\alpha^2 F(\vec{k}, \omega)]\Big|_{\omega=0} = \sum_{\vec{Q}} |M(\vec{k} \to \vec{k} + \vec{Q})|^2 \delta(\epsilon_{\vec{k}+\vec{Q}}) \frac{dB(\vec{Q}, \omega)}{d\omega}\Big|_{\omega=0} , \quad (15)$$

where $(dB/d\omega)|_{\omega=0}$ is zero for noninteracting phonons, but finite when phonon damping is taken into account. Moreover, resonant low-frequency structure in the phonon spectrum, such as has been observed[11] in the high-temperature superconductor Nb_3Sn, will lead to a nonzero value of this quantity and enhance the contributions of Eq. (14) to $1/\tau$. In Sec. IV, an explicit model is used to calculate $\alpha^2 F$ and $1/\tau$ including the effects of phonon damping.

IV. ELECTRON-PHONON-LIMITED PHONON LIFETIMES

The discussion thus far has made use of general properties of the phonon spectral function, independent of the precise mechanism governing phonon decay. We now specialize to the case of electron-phonon-limited phonon lifetimes. This case is particularly simple in several respects. For one thing, estimates of the magnitude of the effect are easily made using sum rules.[12] Another feature of the electron-phonon case is that there is a particularly simple physical picture of the origin of the leading quadratic behavior in T and ω. Figure 1 indicates some important electron and phonon decay processes. Figure 1(a) is Coulomb scattering, where an electron scatters from one momentum state to another, emitting an electron-hole pair. This process is well known from phase-space arguments to lead to ω^2 and T^2 leading behavior for $1/\tau$.[1] Figure 1(b) is the analogous scattering of an electron via the electron-phonon interaction, where a phonon is emitted (or absorbed) instead of the electron-hole pair.

In the process illustrated in Fig. 1(c), an electron scatters by phonon emission (or absorption), but rather than a real phonon, as in Fig. 1(b), a virtual phonon, which subsequently decays by creating an electron-hole pair, is involved. As first noted, to our knowledge, in Ref. 13, this process results in the same decay products as Coulomb scattering [compare Figs. 1(a) and 1(c)], and thus can be expected to have the same phase-space-induced ω^2 and T^2 limitations as Coulomb

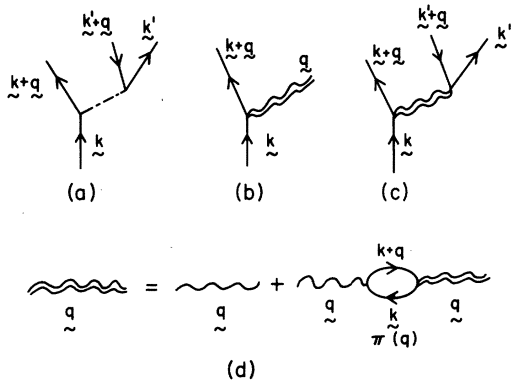

FIG. 1. Illustrating various electron scattering processes. In (a) the initial electron $\vec{k}$ scatters via the Coulomb interaction (depicted by the dashed line). In (b) scattering occurs via emission (or absorption) of a real phonon. In (c) the phonon is virtual, and decays within a time $\hbar/\gamma_{\vec{q}}$ (where $\gamma_{\vec{q}}$ is the phonon width) into an electron-hole pair. There is a close analogy between (a) and (c). However, (c) is already included in the process (b) if the phonons are fully renormalized by their interactions with electrons. This renormalization process is illustrated in (d) which is the Dyson equation. Single wavy lines are bare phonons, and double wavy lines are renormalized phonons. The momenta in all graphs should be regarded as reduced to the first Brillouin zone, and conserved *modulo* a reciprocal lattice vector.

scattering. We present what we believe to be the first quantitative theory of this process, including estimates of the size of the contributions to $1/\tau$. The analysis takes the point of view that the virtual-phonon-mediated process of Fig. 1(c) can be included as a subprocess in a complete treatment of the real-phonon scattering of Fig. 1(b). This leads to simple formulas for the lifetimes. We will find that the subprocess of Fig. 1(c) contributes notably to the total process of Fig. 1 (b) only in the limit of small T and ω. In this limit, the inclusion of phonon decays converts the familiar T^3 or ω^3 behavior of $1/\tau$ into the quadratic forms T^2 and ω^2 more commonly associated with Coulomb scattering. Furthermore, the relative magnitudes of the processes of Figs. 1(a) and 1(b) is fully comparable, just as the dimensionless parameters λ and μ which measure virtual phonon and Coulomb exchange in superconductivity are of roughly equal size. At large T and ω, however, the contribution of Fig. 1(c) drops sharply relative to the Coulomb graph [Fig. 1(a)]. This occurs because of a large energy denominator when the virtual phonon is far off resonance.

In order to calculate the electron-phonon contribution to the phonon lifetime, we use Dyson's equation[1] [shown diagrammatically in Fig. 1(d)] to give the spectral weight function for phonons as

$$B(\vec{Q},\omega)=\frac{1}{\pi}\,\mathrm{Im}\left(\frac{2\Omega_{\vec{Q}}}{\omega^2-\Omega_{\vec{Q}}^2-2\Omega_{\vec{Q}}\,\Pi(\vec{Q},\omega)}\right)\ , \tag{16}$$

where $\Omega_{\vec{Q}}$ is the phonon frequency in the absence of interactions and $\Pi(\vec{Q},\omega)$ is the phonon self-energy. For the electron-phonon case, it is a good approximation (as long as ω is small, of the order of a phonon frequency) to take the real part of Π as constant and the imaginary part as linear in ω. Then with the identifications

$$\omega_{\vec{Q}}^2=\Omega_{\vec{Q}}^2+2\Omega_{\vec{Q}}\Pi_1(\vec{Q},\ \omega_{\vec{Q}})\ , \tag{17a}$$

$$\gamma_{\vec{Q}}=(\Omega_{\vec{Q}}/\omega)\Pi_2(\vec{Q},\omega_{\vec{Q}})\ , \tag{17b}$$

Eq. (16) becomes

$$B(\vec{Q},\omega)=\frac{1}{\pi}\,\frac{\Omega_{\vec{Q}}}{\omega_{\vec{Q}}}\,\mathrm{Im}\left(\frac{2\omega_{\vec{Q}}}{\omega^2-\omega_{\vec{Q}}^2-2i\omega\gamma_{\vec{Q}}}\right)\ . \tag{18}$$

From here on (until Sec. VI) the factor $(\Omega_{\vec{Q}}/\omega_{\vec{Q}})$ will be removed from B and incorporated into the matrix element M^2. Note that the spectral weight function (18) is linear in ω at small frequencies [as anticipated from Eq. (2)]. The result, from Eq. (4), that $F(\omega)$ scales as ω^1 at small ω expresses the fact that a phonon in a metal spends part of its time in the disguise of virtual electron-hole pairs, as shown in Fig. 1(c). It then follows that $\alpha^2F(\vec{k},\omega)$ and $\alpha^2F(\omega)$ must scale as ω^1 in the limit of very small frequencies. In Sec. V, a simple model will be developed to allow detailed calculations of these quantities.

V. EXTENDED DEBYE MODEL

In this section we introduce a model which retains the simplicity of the Debye model but includes the feature that the phonon spectral function $B(\vec{Q},\omega)$ is linear in ω at small ω. In principle, we do not need to identify the mechanism causing the linear behavior. In practice, however, we will only make explicit calculations for the case of the electron-phonon decay mechanism.

The usual Debye model for acoustic phonons consists of a completely isotropic linear dispersion $\omega_{\vec{Q}}=v_s|\vec{Q}|$, where v_s is the velocity of sound. The Brillouin zone is approximated by the Debye sphere of radius $q_D=\omega_D/v_s$. In this approximation, the density of states takes the form

$$F_D^0(\omega)=\sum_{\vec{Q}}\delta(\omega-\omega_{\vec{Q}})=\begin{cases}3\omega^2/\omega_D^3 & (0<\omega<\omega_D)\ ,\\ 0 & (\text{otherwise})\ ,\end{cases} \tag{19}$$

where the subscript D is used to denote Debye and the superscript zero denotes that the phonon lifetime is infinite (B is approximated by a δ function). A simple and fairly realistic extension of this model can be made to include electron-phonon-limited phonon lifetime effects. We make the further assumption

$$\gamma_{\vec{Q}}=\alpha\omega_{\vec{Q}}\ , \tag{20}$$

where α is a dimensionless constant (of order of magnitude 10^{-3} or 10^{-2} in most metals). Equations (18) and (20) together with the usual Debye model, define what we call the "extended Debye model."

The isotropic nature of the model guarantees that $\alpha^2F(\vec{k},\omega)$ is independent of $\vec{k}$ and equal to $\alpha^2F(\omega)$ (provided $\epsilon_{\vec{k}}$ is near the Fermi energy ϵ_F). In general, the function $\alpha^2F(\omega)$ is considerably simpler than $\alpha^2F(\vec{k},\omega)$. The formula (8) can be transformed into a simpler identity,[12]

$$\alpha^2F(\omega)=[\pi N(0)]^{-1}\sum_{\vec{Q}}\frac{\gamma_{\vec{Q}}}{\omega_{\vec{Q}}}\,B(\vec{Q},\omega)\ , \tag{21}$$

where $N(0)$ is the electronic density of states at the Fermi surface for both spin orientations. Within the extended Debye model, Eq. (21) is particularly simple to evaluate. The result is

$$\alpha^2F_D(\omega)=[\alpha/\pi N(0)]F_D^0(\omega)\ . \tag{22}$$

The fact that Eq. (22) explicitly reproduces the observed behavior[5] that α^2F is proportional to F is perhaps the strongest argument in favor of Eq. (20). We feel that Eq. (20) cannot be taken as highly reliable, especially in transition metals, but that it does provide a reasonably good first approximation to real physical systems, while also permitting numerical estimates of electron-phonon effects.

Using the above relations we can express the

phonon density of states including lifetime broadening, F_D^α, as a convolution of the density of states without broadening, F_D^0 and a broadening function of width approximately $\alpha\omega_{\vec{q}}$.

$$F_D^\alpha(\omega)=\frac{1}{\pi}\int_0^\infty d\omega_{\vec{q}}\,F_D^0(\omega_{\vec{q}})\,\mathrm{Im}\left(\frac{2\omega_{\vec{q}}}{\omega^2-\omega_{\vec{q}}^2-2i\alpha\omega\omega_{\vec{q}}}\right). \tag{23}$$

For small α (as occurs in all known metals), the broadened function F_D^α is very similar to the unbroadened function F_D^0, and the two agree in the limit $\alpha\to 0$. The integral in Eq. (23) can be performed analytically, but the precise form is too complicated to be instructive. Figure 2 contains graphs of $\frac{1}{3}\omega_D F_D^\alpha(\omega)$ plotted versus ω/ω_D on logarithmic scales. A reasonable estimate of the value of α for a particular metal can be made from the dimensionless mass-enhancement parameter λ of superconductivity theory.[14] In terms of α^2F, λ is given by

$$\lambda=2\int_0^\infty d\omega\,\alpha^2F(\omega)/\omega\,. \tag{24}$$

If we use Eq. (22), the integral can be done in the extended Debye model. Because α is expected to be small, it is reasonable to approximate $F_D^\alpha(\omega)$ by $F_D^0(\omega)$ when substituting (22) into (24). The result is

$$\lambda\approx 3\alpha/\pi N(0)\hbar\omega_D\equiv\lambda_0\,. \tag{25}$$

The denominator of Eq. (25) is typically 10^{-3}, so α is indeed very small. Thus the parameter λ_0, defined as the right-hand side of Eq. (25), is expected to be very nearly the same as λ. Using Eq. (25) and values of λ quoted by McMillan,[14] approximate values of α are given for various metals in Table I.

TABLE I. Approximate values of α for the extended Debye model calculated from the formula $\alpha=\frac{1}{3}\pi\lambda N(0)\hbar\omega_D$ [Eq. (25)].

Metal	λ[a]	$N(0)$[a] states of both spin per eV per atom	$\hbar\omega_D$[a] (meV)	α
Na	0.15[b]	0.509[b]	13.5	1×10^{-3}
Zn	0.38	0.196	26.6	2×10^{-3}
Al	0.38	0.416	36.2	6×10^{-3}
Pb	1.5[c]	0.55	8.3	8×10^{-3}
Nb	0.82	1.82	23.9	4×10^{-2}
W	0.28	0.30	33.6	3×10^{-3}
Cu	0.22[d]	0.265[d]	26.4	2×10^{-3}

[a]Reference 14 unless otherwise noted.

[b]P. B. Allen and M. L. Cohen, Phys. Rev. 187, 525 (1969).

[c]J. M. Rowell and W. L. McMillan, Phys. Rev. Lett. 14, 108 (1965).

[d]J. F. Janak, Phys. Lett. A 28, 570 (1969).

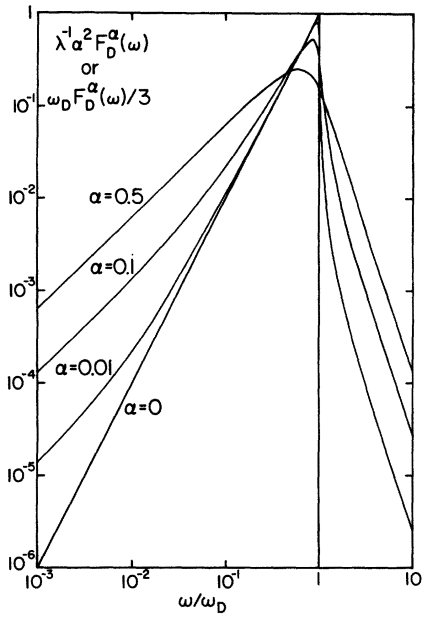

FIG. 2. Phonon density of states in the extended Debye model plotted logarithmically vs the normalized frequency ω/ω_D. The parameter α is a measure of the importance of phonon decay events, being defined as $\gamma_{\vec{q}}/\omega_{\vec{q}}$. The usual Debye curve is realized when $\alpha=0$. Note that the behavior switches from ω^2 to ω^1 at low frequencies when ω/ω_D becomes comparable to α. Values of α as large as 0.1 or 0.5 are not known to occur in nature, but are shown here for illustrative purposes.

The analytic behavior of $\alpha^2F_D^\alpha$ is particularly simple in three limiting cases,

$$\alpha^2F_D^\alpha(\omega)\cong\begin{cases}4\alpha\lambda_0\omega/\pi\omega_D & (\omega\ll\alpha\omega_D)\,,\\ \lambda_0(\omega/\omega_D)^2 & (\alpha\omega_D\ll\omega<\omega_D)\,,\\ 4\alpha\lambda_0\omega_D^3/5\pi\omega^3 & (\omega_D\ll\omega)\,.\end{cases} \tag{26}$$

In the intermediate regime, $\alpha^2F_D^\alpha$ has the familiar Debye-model form; at both high and low frequencies $\alpha^2F_D^\alpha$ acquires tails whose strength is proportional to α. The high-frequency tail apparently gives no observable effects. The low-frequency linear behavior will affect transport coefficients at low T and ω. The crossover between very-low-frequency ω^1 behavior and intermediate-frequency ω^2 behavior occurs at $\omega\sim4\alpha\omega_D/\pi$. The three regimes and the crossover point, which scales as α, can all be seen clearly in Fig. 2.

A similar analysis can be carried out for the temperature dependence of $1/\tau$ by considering various limits of Eq. (12) in the extended Debye model. The results are

$$1/\tau(T)\cong\begin{cases}16\pi^2\lambda_0\alpha\omega_DT^2/3\Theta_D^2 & (T\ll\alpha\Theta_D)\,,\\ 24\pi\zeta(3)\lambda_0\omega_DT^3/\Theta_D^3 & (\alpha\Theta_D\ll T\ll\Theta_D)\,,\\ 2\pi\lambda\omega_DT/\Theta_D & (T\gg\Theta_D)\,,\end{cases} \tag{27}$$

where $\zeta(3)=1.202\ldots$ is the Rieman ζ function. The crossover between the very-low-temperature regime and the intermediate temperature regime occurs when $T=2\alpha\Theta_D/9\zeta(3)$. Analogous results for the frequency dependence of $1/\tau$ are found from Eq. (13)

$$1/\tau(\omega)\cong\begin{cases}4\alpha\lambda_0\omega^2/3\omega_D & (\omega\ll\alpha\omega_D)\,,\\ \pi\lambda_0\omega^3/6\omega_D^2 & (\alpha\omega_D\ll\omega<\omega_D)\,,\\ \frac{2}{3}\pi\lambda_0\omega_D & (\omega\gg\omega_D)\,.\end{cases}\tag{28}$$

The crossover between low- and intermediate-frequency regimes occurs when $\omega=8\alpha\omega_D/\pi$. Graphs of $(\omega_D\tau)^{-1}$ as a function of temperature and frequency are shown on logarithmic scales in Figs. 3 and 4, respectively. For realistic values of α the low-temperature or frequency regime is characterized by such long lifetimes and low temperatures and frequencies that observation of the T^2 or ω^2 behavior will be difficult. However, in the regime where electron-phonon effects behave as T^2 and ω^2, the phonon scattering mechanism is likely to be at least as important as Coulomb scattering (which has occasionally been suspected of being observable). To see this, note that $1/\tau$ in Eqs. (27) and (28) at low T or ω scales as α/ω_D. This parameter can be replaced by

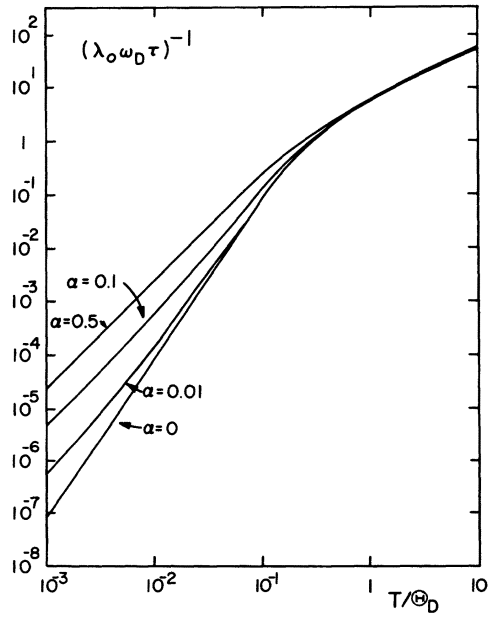

FIG. 3. Temperature dependence of the scattering rate τ^{-1} normalized to $\lambda_0\omega_D$ in the extended Debye model, for various values of the phonon decay parameter α. When α is zero, the usual Debye model T^3 behavior occurs at small T. For nonzero α, the low-T behavior is $\alpha(T/\Theta_D)^2$. When T is roughly $\alpha\Theta_D/5$, the curves change from T^2 to T^3.

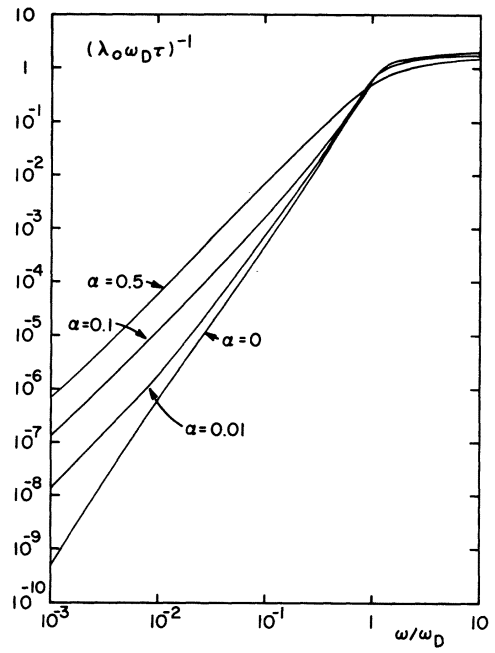

FIG. 4. Frequency dependence of the scattering rate τ^{-1} normalized to $\lambda_0\omega_D$ in the extended Debye model, for various values of the phonon decay parameter α. When α is zero, the usual Debye model ω^3 behavior occurs at small ω. For nonzero α, the low-ω behavior is $\approx\alpha(\omega/\omega_D)^2$. When ω is roughly $\alpha\omega_D$, the curves change from ω^2 to ω^3.

$\frac{1}{3}\pi\lambda_0N(0)\hbar$ according to Eq. (25). Then we can combine Eqs. (27) and (28) to obtain

$$1/\tau(\omega,T)\cong4\pi\lambda_0^2N(0)[(\hbar\omega)^2+(2\pi k_BT)^2]/9\hbar$$
$$(T\ll\alpha\Theta_D,\quad\omega\ll\alpha\omega_D)\,,\tag{29}$$

which is the explicit evaluation of Eq. (14) for the case of electron-phonon-limited phonon lifetimes. A reasonable estimate of the strength of Coulomb scattering would entail replacing λ_0^2 in Eq. (29) by μ^2 where μ is the dimensionless measure of Coulomb repulsion used in superconductivity theory. Typically λ and μ are about the same size in metals, although in monovalent metals λ is quite a bit smaller than μ; and in good superconductors λ is quite a bit larger. Therefore, if a T^2 or ω^2 behavior of $1/\tau$ is to be sought after, the phonon mechanism is just as good a candidate as the Coulomb mechanism. In fact, the largest effect would be expected to be the phonon effect in a good superconductor like Pb or Nb.

Finally, it is worth mentioning that the quasiparticle lifetime $\tau(\epsilon,T)$ for an electron of known energy ϵ, as given by Eq. (9), can be written at very low T and ω in the extended Debye model:

$$1/\tau(\epsilon,T)=4\pi\lambda_0^2N(0)[\epsilon^2+(\pi k_BT)^2]/3\hbar\,.\tag{30}$$

The factor $\epsilon^2+(\pi k_B T)^2$ is familiar in Fermi-liquid theory.[1] The observable lifetime, when averaged over available energies in the manner of Eq. (10). has the form of Eq. (29) instead of (30). Thermal averaging enhances the temperature-dependent scattering rate by 4/3 over the value in Eq. (30) which is appropriate for electrons right at the Fermi surface. This occurs because electrons $k_B T$ away from the Fermi surface also contribute and have faster scattering rates. On the other hand, at nonzero frequency ω, but $T=0$, the observable scattering rate is *smaller* than that given by Eq. (30), by a factor of $\frac{1}{3}$. This occurs because all electrons in the range $|\epsilon| < \omega$ are probed rather than simply those with $|\epsilon| = \omega$ which have the shortest lifetimes. These conclusions are equally valid for Coulomb scattering. Analogous averaging effects[9,10,15] occur in the (T^3, ω^3) electron-phonon regime, but the numerical factors are different.

VI. MASS ENHANCEMENT AND SUPERCONDUCTIVITY

The parameter λ defined in Eq. (24) is an important dimensionless measure of the electron-phonon coupling. In superconductors[14] λ plays the role of the Bardeen-Cooper-Schrieffer[16] (BCS) parameter $N(0)V$, while in normal metals[1] $1+\lambda$ occurs as the mass enhancement which is observed in specific-heat or cyclotron-resonance measurements. We are now in a position to make some general remarks on the question of how λ is affected by including the dynamical interactions of the phonons, rather than treating them as infinitely sharp excitations.

If the δ-function approximation is used for B, then Eqs. (7), (8), and (24) can be combined, giving

$$\lambda = N(0)\langle\langle |M(\vec{k}-\vec{k}')|^2/\hbar\omega_{\vec{k}-\vec{k}'}\rangle\rangle \ , \tag{31}$$

where the angular brackets indicate averaging $\vec{k}$ and $\vec{k}'$ over the Fermi surface, i.e.,

$$\langle\langle g(\vec{k},\vec{k}')\rangle\rangle \equiv \sum_{\vec{k},\vec{k}'} g(\vec{k},\vec{k}')\delta(\epsilon_{\vec{k}})\delta(\epsilon_{\vec{k}'}) \Big/ \sum_{\vec{k},\vec{k}'} \delta(\epsilon_{\vec{k}})\delta(\epsilon_{\vec{k}'}) \ . \tag{32}$$

When the full dynamical nature of $B(\vec{Q},\omega)$ is taken into account, the integral (24) can no longer be evaluated by simply using the peak frequency $\omega_{\vec{k}-\vec{k}'}$ of the spectral function. However, the integral can be done formally, using the identity

$$\int_0^\infty (d\omega/\omega)B(\vec{Q},\omega) = -\tfrac{1}{2}D(\vec{Q},0) \ . \tag{33}$$

This relation between the spectral weight function B and the static Green's function (or lattice displacement-displacement correlation function, or susceptibility) follows trivially from Eq. (1), using the fact that B is odd in ω. Using Dyson's equation [see Eq. (16)], the static Green's function is

$$-\tfrac{1}{2}D(\vec{Q},0) = \Omega_{\vec{Q}}/[\Omega_{\vec{Q}}^2 + 2\Omega_{\vec{Q}}\Pi_1(\vec{Q},0)] \ . \tag{34}$$

It is conventional to define a frequency, $\omega_{\vec{Q}}(0)$, which describes the frequencies that the phonons would have if $\Pi_1(\vec{Q},\omega)$ were frequency independent (i.e., if the restoring force at the phonon frequency were the same as the restoring force to static deformations). Thus,

$$\omega_{\vec{Q}}^2(0) = \Omega_{\vec{Q}}^2 + 2\Omega_{\vec{Q}}\Pi_1(\vec{Q},0) \ . \tag{35}$$

The frequency $\omega_{\vec{Q}}(0)$ differs from the experimental frequency $\omega_{\vec{Q}}$ which is defined as the frequency at which the phonon spectral function peaks. If $\Pi_2(\vec{Q},\omega)$ varies slowly with ω, then the experimental frequency $\omega_{\vec{Q}}$ is defined by Eq. (17a). Usually the frequencies defined by Eqs. (35) and (17a) have been regarded as equivalent for metals at low temperatures. If Π arises from electron-phonon interactions only, then equality between (35) and (17a) is a statement of the adiabatic approximation. The pseudopotential method[17] for calculating phonon spectra has been shown[18] to be equivalent to using (35). However, in principle, (17a) is the more meaningful frequency, and there is no reason why (35) and (17a) should agree in more complicated situations (such as alloys). In fact, in Nb_3Sn, an important high-T_c material, recent experiments[11] have shown (17a) to differ markedly from (35) for certain phonons, namely, the $\langle 110\rangle$ TA branch associated with the 40 °K structural transformation. In this case $\omega_{\vec{Q}}(0)$ is quite a lot smaller than $\omega_{\vec{Q}}$ because the spectral function B is observed to contain a "central peak" in addition to the usual phonon sidebands.

If we use the results [Eqs. (33)–(35)] to recompute λ for the general case of an arbitrary spectral function, we find

$$\lambda = N(0)\langle\langle |M_0(\vec{k}-\vec{k}')|^2/\hbar\omega_{\vec{k}-\vec{k}'}(0)\rangle\rangle \ . \tag{36}$$

Thus, we have the interesting result that λ is determined by the static frequency $\omega_{\vec{Q}}(0)$ rather than the measured peak frequency $\omega_{\vec{Q}}$. The subscript zero on the matrix element M in (36) is meant to indicate that the static frequency $\omega_{\vec{Q}}(0)$ should be used in computing the displacement $\delta R_{\vec{Q}} = [\hbar/2MN\omega_{\vec{Q}}(0)]^{1/2}$ which enters M. Thus λ depends on $\omega_{\vec{Q}}(0)$ raised to the inverse second power. This observation might lead one to believe that the peculiar line shape observed by Shirane and Axe[11] for $\langle 110\rangle$ TA phonons in Nb_3Sn would result in an enhancement of λ, which would have important consequences in raising T_c. The fact that experimental values of $\gamma_{\vec{Q}}$ are also available for these phonons[19] provides hope that the contribution to $\alpha^2F(\omega)$ arising from these phonons can be numerically evaluated using Eq. (21). However, such a program is not possible yet because of uncertainty in the measured values of $\gamma_{\vec{Q}}$ and dif-

ficulties in knowing how to extrapolate $\gamma_{\vec{Q}}$ off symmetry directions. Nevertheless, we believe that Nb_3Sn must have an unusually large linear term (in ω) in $\alpha^2F(\omega)$ arising from these soft and peculiar phonons. However, a convincing argument can be made against the speculation that λ and, thus, T_c would be enhanced. Certainly λ could be increased, but the effect of this on superconductivity would be much less than a naive application of McMillan's[14] equation would suggest. The ineffectiveness of low-frequency phonons in raising T_c is omitted in McMillan's simplified treatment, but has been described by Barisic[20] and calculated in more detail by Allen[21] and by Bergmann and Rainer.[22]

In addition to the integral (24) which defines λ, there is another integral over α^2F which defines a mean-square frequency $\langle\omega^2\rangle$ of importance to superconductivity, Thus,

$$\lambda\langle\omega^2\rangle \equiv 2\int_0^\infty d\omega\,\omega\alpha^2F(\omega)\,. \tag{37}$$

This integral was shown by McMillan[14] (for infinitely sharp phonons) to be dependent only on the atomic mass M and the electronic properties of the solid, i.e., independent of the phonon spectrum. It is easily shown that the integral (37) is totally unaffected by the form of the phonon spectral function $B(\vec{Q},\omega)$. This follows from the well-known sum rule[4]

$$\int_0^\infty d\omega\,\omega B(\vec{Q},\omega) = \Omega_{\vec{Q}}^2. \tag{38}$$

This result holds for the true spectral function, as well as for the δ-function approximation. Recently, Taylor and Vashishta[23] have exploited the sum rule (38) and a variant of (33) in order to discuss the superconductivity of alloys.

As a final point, we discuss some implications of the low-ω linear behavior of $\alpha^2F(\omega)$ on the temperature dependence of the mass enhancement, specific heat, and other thermodynamic quantities. It was first pointed out by Eliashberg[24] that the mass enhancement can lead to higher-order terms in the temperature dependence of the electronic specific heat. Specifically, if we write

$$C_{el} = \gamma T = \tfrac{1}{3}\pi^2N(0)(1+\lambda)k_B^2T\,, \tag{39}$$

then λ will have a temperature dependence. Eliashberg's leading behavior was of the type

$$\lambda = \lambda_0 + \lambda_1T^2\ln(\Theta_D/T)\quad(\lambda_1>0)\,. \tag{40}$$

This result follows if quadratic behavior is assumed for $\alpha^2F(\omega)$ at low ω. However, Allen and Cohen[25] pointed out that behavior of the type

$$\lambda = \lambda_0 - \lambda_2T^2\quad(\lambda_2>0) \tag{41}$$

would occur if $\alpha^2F(\omega)$ were linear in ω. Behavior of the type (40) has been observed for a number of metals,[26] although λ_1T^2 fits the data as well as $\lambda_1T^2\ln(\Theta_D/T)$. Furthermore, the effect is not directly visible in the specific heat and has been seen only in Azbel-Kaner resonance where the theory gives similar expressions.[9,27] At low enough temperatures, however, the form (41) must always hold.

Direct measurement of specific heat does not reveal (40) or (41) because higher-temperature behavior is dominated by the lattice specific heat. However, the electronic specific heat is related thermodynamically to the superconducting critical field. Lambert[28] has seen indirect evidence for (40) in the critical field of mercury. Very large linear terms in α^2F occur in amorphous materials, as previously mentioned. Bergmann[29] has presented evidence for behavior of the form (41) in such materials.

Note added in proof. Professor T. Holstein has kindly pointed out to us that the electron-phonon-induced quadratic behavior of τ^{-1} on ϵ was in fact first discussed by Migdal.[3] Equations (30) and (31) of Ref. 3 are basically equivalent to Eq. (28) of the present paper. Professor Holstein has also discussed this effect.[30]

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[1]For general reviews, see J. R. Schrieffer, *Superconductivity* (Benjamin, New York, 1964); D. J. Scalapino, in *Superconductivity*, edited by R. D. Parks (Dekker, New York, 1969); J. W. Wilkins, *Observable Many Body Effects in Metals* (Nordita, 1968).

[2]W. L. McMillan and J. M. Rowell, in *Superconductivity*, edited by R. D. Parks (Dekker, New York, 1969).

[3]A. B. Migdal, Zh. Eksp. Teor. Fiz. 34, 1438 (1958) [Sov. Phys.-JETP 7, 996 (1958)].

[4]R. A. Cowley, in *Phonons in Perfect Crystals and in Lattices with Point Imperfections*, edited by R. W. H. Stevenson (Plenum, New York, 1966).

[5]J. M. Rowell and R. C. Dynes, in *Phonons*, edited by

M. A. Nusimovici (Flammarion, Paris, 1971), p. 150.
[6]T. T. Chen, J. T. Chen, J. D. Leslie, and H. J. T. Smith, Phys. Rev. Lett. 22, 526 (1969); K. Knorr and N. Barth, Solid State Commun. 8, 1085 (1970).
[7]H. Scher and T. Holstein, Phys. Rev. 148, 598 (1966).
[8]J. M. Ziman, *Electrons and Phonons* (Oxford, London, 1960).
[9]P. B. Allen, *Proceedings of the Twelfth International Conference on Low Temperature Physics*, edited by E. Kanda (Keigaku, Tokyo, 1971), p. 517.
[10]P. B. Allen, Phys. Rev. B 3, 305 (1971). Factor of 2 errors in this paper have been corrected in the present work.
[11]G. Shirane and J. D. Axe, Phys. Rev. Lett. 27, 1803 (1971).
[12]P. B. Allen, Phys. Rev. B 6, 2577 (1972).
[13]E. W. Fenton, J.-P. Jan, A. Karlsson, and R. Singer, Phys. Rev. 184, 663 (1969), and references therein.
[14]W. L. McMillan, Phys. Rev. 167, 331 (1968).
[15]P. B. Allen (unpublished).
[16]J. Bardeen, L. N. Cooper, and J. R. Schrieffer, Phys. Rev. 108, 1175 (1957).
[17]For a recent review, see V. Heine and D. L. Weaire, in *Solid State Physics*, edited by H. Ehrenreich *et al.* (Academic, New York, 1970), Vol. 24.
[18]P. N. Keating, Phys. Rev. 175, 1171 (1968); L. J. Sham, Phys. Rev. 188, 1431 (1969); R. M. Pick, M. H. Cohen, and R. M. Martin, Phys. Rev. B 1, 910 (1970).
[19]J. D. Axe and G. Shirane, Phys. Rev. Lett. 30, 214 (1973).
[20]S. Barisic, Phys. Rev. B 5, 932 (1972).
[21]P. B. Allen, Solid State Commun. (to be published).
[22]G. Bergmann and D. Rainer, Z. Phys. 263, 59 (1973).
[23]D. W. Taylor and P. Vashishta, Phys. Rev. B 5, 4410 (1972).
[24]G. M. Eliashberg, Zh. Eksp. Teor. Fiz. 43, 1005 (1962) [Sov. Phys.-JETP 16, 780 (1963)].
[25]P. B. Allen and M. L. Cohen, Phys. Rev. B 1, 1329 (1970).
[26]J. J. Sabo, Jr., Phys. Rev. B 1, 1325 (1970).
[27]G. Grimvall, J. Phys. Chem. Solids 29, 1221 (1968).
[28]M. Lambert, Phys. Rev. B 3, 4416 (1971).
[29]G. Bergmann, *Proceedings of the Thirteenth International Conference on Low Temperature Physics, Boulder, Colo.*, 1972, edited by R. H. Kropschot and K. D. Timmerhaus (University of Colorado Press, Boulder, Colo., 1973).
[30]T. Holstein, Ann. Phys. (N.Y.) 29, 410 (1964).