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Generalization of the theory of the electron-phonon interaction: Thermodynamic formulation of superconducting- and normal-state properties

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A thermodynamic formulation for the electron self-energy is given which is applicable when the electronic spectrum possesses structure on the scale of phonon frequencies, provided only that the ratio of phonon phase velocity to electron Fermi velocity is small. Electron-phonon, Coulomb, and electron-defect interactions are included on an equal footing and it is shown that their different frequency dependencies lead to specific effects on the Eliashberg self-energy: (a) The Coulomb interaction contributes nothing of essence to the normal-state self-energy (in this isotropic approximation) but retains its usual depairing effect upon the superconducting gap function, (b) defects affect superconducting properties primarily through a broadening of the electronic spectrum, and (c) phonons contribute a thermal shift and broadening as well as the mass enhancement. A generalization to *intensive* electron-phonon, electron-electron, and electron-defect interaction constants is necessary to redevelop an intuition into the effects of these interactions. The change in the structure of the Eliashberg equation due to a nonconstant density of states (DOS) and the consequent interplay between static and thermal disorder is analyzed in detail, with a central feature being the change in frequency dependence of the self-energy compared to a constant DOS solution. The effect of DOS structure on the superconducting transition temperature T_c, which is manifested in the defect dependence of T_c, is analyzed in detail. Further it is proposed that an extension of the self-consistent Eliashberg approach be extended above T_c to determine the normal-state self-energy and thereby the electronic contribution to thermodynamic quantities. Phonon broadening is shown to affect the spin susceptibility at finite temperature. Reinterpretation of several of the anomalous properties of $A15$ compounds in terms of the present theory is suggested. Several aspects of the theory are compared to experimental data for Nb_3Sn.

I. INTRODUCTION

Deeply ingrained in the formal theory of the interacting electron-phonon (*e*-ph) system in metals are two simplifying approximations. The first is an extension of the adiabatic, or Born-Oppenheimer approximation[1] in which the light electrons are considered to respond instantaneously to the heavy ions (of mass M). Central to the theory of *e*-ph systems is Migdal's theorem,[2] which demonstrates that nonadiabatic effects can be obtained accurately by low-order Feynman-Dyson perturbation theory, to lowest order in an expansion parameter of the order of $(m/M)^{1/2} \ll 1$. The second simplification is the assumption of a constant density of states (CDOS) over a region $\pm\overline{\Omega}$ around the Fermi energy E_F, where $\overline{\Omega}$ is a few times of the mean phonon frequency. This approximation allows the DOS function $N(E)$ to be approximated by $N(E_F)$ in certain energy integrals. The two approximations in fact are related, and it often seems to be assumed that Midgal's theorem is inapplicable if $N(E)$ is not constant [to within $(m/M)^{1/2}$] over a range $\pm\overline{\Omega}$ around E_F. As will be shown in this paper, however, there exists an important regime within which the CDOS approximation may be relaxed in a straightforward manner while retaining Migdal's simplification. The resulting generalizations of the CDOS expressions often are not intuitively obvious, and the consequences involve a reinterpretation of many of the properties of this class of materials.

That structure in the DOS on the scale of $\overline{\Omega}$ should be expected in crystals containing several transition-metal atoms per unit cell can be deduced from general considerations.[3] Elemental transition metals are known to have peak structure in their DOS which may be only a few tenths of an eV wide. A compound with (for example) ten atoms per unit cell will have 10 times the number of bands in the same overall bandwidth, leading to structure on the order of hundredths of an eV.

Recent band-structure calculations[4,5] on $A15$ compounds (eight atoms per unit cell) indeed have verified structure on this scale. DOS structure can be important even in elemental metals if the Fermi level E_F lies near a van Hove singularity, such as occurs in Pd and Pt.

The most intriguing consequence of the e-ph interaction, both theoretically and technologically, is superconductivity, and it has not been overlooked that the superconducting transition temperature T_c might be affected by DOS fine structure. An early study of $A15$ compounds was carried out by Barisič and co-workers[6] in the weak-coupling limit, where it was noted that the DOS within a region $\pm\overline{\Omega}$ around E_F contributes in the determination of T_c. Cohen, Cody, and Vieland[7] applied a strong-coupling version of the Koonce-Cohen[8] formalism to investigate the effect of model $A15$ DOS functions upon T_c.

In a model solution of the Eliashberg equation with non-CDOS effects included approximately Nettel and Thomas[9] suggested an average DOS given by

$$\overline{N}_{\mathrm{NT}}=\frac{1}{2}\int_{T_c}^{\Omega_c}\frac{d\omega}{\omega Z(\omega)}\times[N(\omega Z)+N(-\omega Z)]/\ln(\Omega_c/T_c) \tag{1.1}$$

as being most relevant in determining T_c. Here $Z(\omega)$ is the strong-coupling renormalization (real part), $\Omega_c \approx \overline{\Omega}$ is a cutoff frequency, and the DOS function will be taken with origin at E_F throughout this paper. It was evident to Nettel and Thomas that there is great utility in identifying, whenever possible, an effective value of $N(E_F)$ for use in the CDOS version of Eliashberg theory rather than having to deal always with the full energy dependence explicitly. This simplication will be explored further in this paper.

Horsch and Rietschel[10] obtained numerical solutions to the Eliashberg equation in the small $kT_c/\overline{\Omega}$ limit where the imaginary part of the self-energy can be neglected. They found an enhancement of T_c relative to the CDOS value T_c^0 for placements of a square root DOS peak near $E_F-\overline{\Omega}Z(0)$. This was interpreted as a reduction of the repulsive part of the e-ph interaction due to DOS variation. It could equally well be considered as an enhancement of the attractive part of the interaction (which occurs at $\omega<\overline{\Omega}$), with an approximate value of the enhancement given by $\overline{N}_{\mathrm{NT}}$.

A more general approach was taken by Lie and Carbotte,[11] who calculated a functional derivative $\delta T_c/\delta N(E)$ for several superconductors. Its shape was found to be quite insensitive to the metal considered, having a maximum at $E=E_F$, decreasing to half maximum at

$$|E-E_F| \approx 5-10T_c$$

and becoming negative (but remaining very small) above

$$|E-E_F| \approx 50-70T_c \ .$$

This (linear) approach leads to an average DOS

$$\overline{N}_{\mathrm{LC}}=\int dE\frac{\delta T_c}{\delta N(E)}N(E)\Big/\frac{dT_c}{dN(E_F)} \tag{1.2}$$

which is useful for estimating T_c from a CDOS theory. In Eq. (1.2) $dT_c/dN(E_F)$ is the integral over $\delta T_c/\delta N(E)$, and T_c is given by

$$T_c=T_c^0+[\overline{N}_{\mathrm{LC}}-N(E_F)]\frac{dT_c}{dN(E_F)} \ . \tag{1.3}$$

Written in this form $\overline{N}_{\mathrm{LC}}$ clearly has an interpretation as an effective value of $N(E_F)$. Since the important contributions to the integral in Eq. (1.2) come from the region $|E-E_F|<10T_c \sim \Omega_c$ (for strong coupling superconductors), for nonpathological DOS functions the averages $\overline{N}_{\mathrm{NT}}$ and $\overline{N}_{\mathrm{LC}}$ should be similar.

Whereas an average over the DOS may be sufficient for understanding T_c, for many properties of interest (e.g., the T dependence of the spin susceptibility χ_{sp}) no such simplification will be possible. In this paper a general approach for obtaining the electronic self-energy, and thereby the thermodynamic properties, is described. Both static and dynamic disorder are included in a straightforward generalization[12] of the usual Eliashberg approach, and it is shown that each type of disorder contributes to the shift in chemical potential as well as to a shift and renormalization of the electronic spectrum. Although the emphasis here will be focused on the superconducting state, implications for normal-state properties also will be discussed. A preliminary report[13] of the application of this theory to $\mathrm{Nb_3Sn}$ has been published elsewhere.

The plan of the paper is as follows. Section II is devoted to the description of the system of interacting electrons, phonons, and defects which will be studied, and the approximations leading to our expression for the electronic self-energy are discussed and justified. The treatment of the energy dependence in the Eliashberg equation is given in Sec. III, where it is argued that the band-energy dependence of the self-energy should be negligible in most cases. This leads in turn to a less formidable numerical procedure for solving for the self-energy. In Sec. IV the generalized Eliashberg system of equations is presented and the alterations arising from DOS structure are discussed. As a byproduct of retaining the band-energy dependence of the e-ph interaction in the equations, a better understanding of the Coulomb pseudopotential and of the role of impurity scattering is obtained. A discussion of several aspects of the theory at T_c is presented in Sec. V. In Sec. VI the spin susceptibility is discussed in terms of a self-energy determined from an Eliashberg-type equation at $T > T_c$. Unlike previous uses of Eliashberg-type equations,[14] which of necessity require an infinite summation of diagrams to describe appropriately the appearance of a gap (superconducting or spin-density-wave) in the spectrum, this novel application accomplishes more easily what could be accomplished (at least approximately) in some finite order of perturbation theory. It is suggested that this approach may be fruitful for studying other thermodynamic properties. Indeed, there has been little concern over non-CDOS corrections above T_c with the exception of the T dependence of χ_{sp} and the elastic constants, both of which show anomalous behavior in high-T_c $A15$ compounds.

II. GENERALIZATION OF THE ELIASHBERG SELF-ENERGY

The usual treatment of Eliashberg theory on the imaginary frequency axis is clearly set forward in the literature.[15] We will provide only the background necessary to clarify the generalizations we propose and the approximations which remain. The system we consider is described by the Hamiltonian

$$H = H_e + H_{\text{ph}} + H_{e\text{-}e} + H_{e\text{-ph}} + H_{\text{imp}} \ , \tag{2.1a}$$

where

$$H_e = \sum_k E_k \Psi_k^\dagger \tau_3 \Psi_k \ , \tag{2.1b}$$

$$H_{\text{ph}} = \sum_{Q\nu} \Omega_{Q\nu} b_{Q\nu}^\dagger b_{Q\nu} \ , \tag{2.1c}$$

$$H_{e\text{-}e} = \tfrac{1}{2} \sum_{kkq} V(k,k';q) \Psi_{k-q}^\dagger \tau_3 \times \Psi_k \Psi_{k'+q}^\dagger \tau_3 \Psi_{k'} \ , \tag{2.1d}$$

$$H_{e\text{-ph}} = \sum_{k,k',\nu} g_{kk'\nu}(b_{k-k',\nu}^\dagger + b_{k'-k,\nu}) \times \Psi_{k'}^\dagger \tau_3 \Psi_k + \mathscr{T} \ , \tag{2.1e}$$

$$H_{\text{imp}} = \sum_{kk'} \sum_{j=1}^{n_i} V_{kk}^{\text{imp}}(R_j) \Psi_k^\dagger \tau_3 \Psi_k \ , \tag{2.1f}$$

where $\mathscr{T}$ denotes a second-order term. In the Nambu scheme the spin index is eliminated in favor of the two-component field operator

$$\Psi_k = \begin{bmatrix} c_{k\uparrow} \\ c_{-k\downarrow}^\dagger \end{bmatrix} \tag{2.2}$$

in terms of the electron annihilation operator $c_{k\sigma}$. The Pauli matrices are denoted by τ_1, τ_2, and τ_3. Electron-band and phonon-mode indices will not be exhibited explicitly except where necessary.

In this form of the Hamiltonian Ψ describes *band electrons*, for which the electron-static lattice and electron-electron interactions have been included in a mean-field sense. For the electron-lattice interaction the remaining coupling is given, to second order in the ion displacement, by the electron-phonon Hamiltonian $H_{e\text{-ph}}$. The second-order term, which has not been displayed explicitly, is required to keep the theory translationally invariant.[16] The residual Coulomb interaction between band electrons is assumed to be representable in the usual four-body form and is denoted by V in the electron-electron Hamiltonian $H_{e\text{-}e}$. The effect of this term on superconducting behavior is not understood in detail but fortunately an approximate treatment in terms of an empirical "Coulomb pseudopotential" (see below) seems sufficient for most purposes.

The "impurity" term H_{imp} represents[17] n_i identical, randomly distributed imperfections centered at positions R_j. The scattering potential V^{imp} represents the *difference* between the potential in the region of the imperfection and the perfect-crystal potential. The phonon Hamiltonian H_{ph} is expressed in terms of bare phonons (with creation operator $b_{Q\nu}^\dagger$) of frequency $\Omega_{Q\nu}$, which are dressed to the observed frequency $\omega_{Q\nu}$ by the band-electron polarization as described for example by Migdal.[2] In this paper we will *not* consider the effect of lattice imperfections on either the phonon spectrum or the electron-phonon coupling g, although the effect may become large for highly disordered materials.

The electron thermodynamic Green's function is given by

$$G(k,i\omega_n)^{-1}=i\omega_n-(E_k-\zeta)\tau_3-\Sigma(k,i\omega_n)\,, \tag{2.3}$$

where $\omega_n=(2n+1)\pi T$ and the self-energy Σ conventionally is given by[15]

$$\Sigma(k,i\omega_n)=i\omega_n[1-Z(k,i\omega_n)] +\chi(k,i\omega_n)\tau_3+\phi(k,i\omega_n)\tau_1\,. \tag{2.4}$$

For bulk superconducting properties the τ_2 term in Σ is proportional to ϕ and is assumed to be eliminated by the choice of phase. Two points should be noted here. First, the chemical potential ζ, which is determined by the relation

$$N_e=T\sum_{k,n}\mathrm{Tr}G(k,i\omega_n)e^{i\omega_n\epsilon} \tag{2.5}$$

in terms of the number of electrons N_e (ϵ is a positive infinitesimal quantity), will be retained explicitly. Second, we also retain the energy shift χ (not to be confused with the susceptibility) and find that although it does not reduce to a trivial shift in the chemical potential, its effects are usually of a secondary nature.

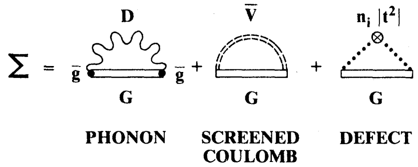

FIG. 1. Proposed phonon, Coulomb, and defect contributions to the electron self-energy Σ. The double lines indicate the renormalized Green's function $G(\Sigma)$, giving a self-consistent, infinite order relation for Σ.

The Eliashberg equation for the self-energy, represented diagramatically in Fig. 1 is[15]

$$\Sigma(k,i\omega_n)=-T\sum_{k',n'}\tau_3G(k',i\omega_{n'})\tau_3\left[\sum_{\nu}|\bar{g}_{kk'\nu}|^2D_\nu(k-k',i\omega_n-i\omega_{n'}) +\bar{V}(k,k';i\omega_n-i\omega_{n'})+[n_i\,|t(k,k',i\omega_n)|^2/T]\delta_{nn'}\right]. \tag{2.6}$$

The first term results from coupling to phonon branch ν with renormalized phonon Green's function D_ν. The second term arises from the dynamically screened and Coulomb-vertex-corrected electron-electron interaction $\bar{V}$, which is discussed further below. The third term, which is usually not included, results from neglecting *correlated* multiple scattering between distinct static defects, but includes multiple scattering from a single defect by means of the t matrix[17] t. This treatment strictly applies to the dilute limit; however, the transport theory which results usually is found to be valid to rather large defect concentrations.

In writing the phonon contribution to Σ as in Eq. (6), Migdal's theorem[2] has been invoked. In its usual form this theorem states that, to within a quantity of order $(m/M)^{1/2}$, the electron-phonon vertex function $\Gamma_{e\text{-ph}}$ can be taken as unity (for the purpose of calculating the electron self-energy). Within simple metal language an equivalent expansion parameter is $\bar{\Omega}/E_f$. This had led to speculation that Migdal's theorem may not hold for systems which have DOS structure, and in some sense an effective degeneracy temperature (E_F) on the scale of $\bar{\Omega}$. As Scalapino[15(c)] has emphasized, however, the validity of the approximation rests on a small value of the ratio of phonon phase velocity ω_Q/Q to electron group velocity v_k. Even for *A* 15 compounds with large $N(E_f)$ and low electron velocities the ratio of these quantities averaged over the Brillouin zone is $(2-3)\times10^{-2}$ (e.g.,[18] $\langle\omega_Q/Q\rangle\sim5\times10^5$ cm/sec and[5] $\langle v_k\rangle\simeq\langle v_k^2\rangle^{1/2}\equiv v_F=2\times10^7$ cm/sec for $\mathrm{Nb_3Sn}$). The approximation $\Gamma_{e\text{-ph}}=1$ can break down in the *immediate* vicinity of a van Hove singularity $v_k=0$, but such a small number of electrons within $|E_k-E_f|<\bar{\Omega}$ have $v_k\lesssim\omega_Q/Q$ that the contribution to the Brillouin-zone sum in Eq. (2.6) will be negligible.

Recently Drozhov[19] has provided more insight into this problem. The situation Drozhov studied is that in which an M_1 van Hove critical point falls at E_F, which is one situation for which $v_k\leq\omega_Q/Q$. It was found that so much dispersion is introduced into the electronic states by the e-ph interaction that the corresponding quasiparticles are for the most part removed from the region of the critical point (and, of course, are highly damped). The quasiparticle velocities tend to diverge at the critical point. Thus, if the fully renormalized Green's function, rather than its bare counterpart, is used in Eq. (2.6) (as is done in Eliashberg theory and as it is shown in later sections must also be done in the normal state), it may well be the case that the criterion $V_k\geq\omega_Q/Q$

in terms of *renormalized velocities* V_k (if they can be defined) is satisfied even near critical points $v_k \rightarrow 0$ where Migdal's theorem as stated is unproven. Assuming this to be the case, the only remaining difficulty is with optic modes, for which near zone-center phase velocities ω_Q/Q diverge. It appears that a small enough number of modes are involved that the Brillouin-zone sum for Σ is unaffected.

Migdal[2] also demonstrated (for the normal state at $T=0$) that the renormalized Green's function G appearing on the right-hand side of Eq. (2.6) can be replaced, in the CDOS system he considered, by the unrenormalized Green's function, thus allowing a formal solution for low frequencies. No corresponding simplification is possible when variation in $N(E)$ is not negligible, as observed by Eliashberg[15(h)] for the superconducting state in which the opening of the gap gives a sharply varying density of quasiparticle states. A central point of this paper is that, when the energy variation of $N(E)$ occurs on the scale of phonon energies, Σ must be determined self-consistently from Eqs. (2.5) and (2.6) for the normal state as well.

The three contributions to Σ in Eq. (2.6) differ fundamentally in their frequency dependence. The phonon Green's function $D_\nu(i\omega_n)$ has its important frequency variation for $|\omega_n| \lesssim \overline{\Omega}$ and decreases as ω_n^{-2} for $|\omega_n| \gg \overline{\Omega}$. The Coulomb interaction $\overline{V}(i\omega_n)$ varies only on the scale of the electronic plasma frequency (peak in the energy-loss function) $\omega_{\mathrm{pl}} \sim 10$ eV. The impurity contribution is energy conserving, with $(1/T)\delta_{n,n'}$ in Eq. (2.6) representing the δ function $\delta(\omega-\omega')$ in the thermodynamic formulation. For the phonon and impurity contributions the sum over $|\omega_{n'}|$ in Eq. (2.6) can be truncated at a cutoff frequency $\omega_c \sim 5-10\overline{\Omega}$ with negligible loss of accuracy. The practical necessity of using a minimal frequency range for solving for Σ has prompted the folding down of the Coulomb potential $\overline{V}$ into a pseudopotential $\overline{U}$ as described in detail elsewhere.[15,20] The treatment is generalized somewhat in Appendix A, with the result

$$1/\overline{U} = 1/\overline{V} + \overline{N}(\omega_{\mathrm{pl}})\ln(\omega_{\mathrm{pl}}/\omega_c)\ . \tag{2.7}$$

This relation, and the effective DOS $\overline{N}(\omega_{\mathrm{pl}})$, will be discussed further in Sec. IV A. Using this pseudopotential and utilizing the evenness[15(b)] in frequency ω_n of the functions Z, χ, and ϕ, Eq. (2.6) can be reduced to an $N_c \times N_c$ matrix equation with $(2N_c-1)\pi T = \omega_c$ (i.e., $n=0,1,\ldots,N_c-1$).

III. TREATMENT OF THE ENERGY DEPENDENCE

In its most general form the Eliashberg equation is extremely difficult to solve even if the kernel in large parentheses in Eq. (2.6) is known. Besides the four-dimensional frequency-momentum variables which are summed over, G and Σ also are matrices in band index,[21] although this fact is nearly always ignored. To date little of a quantitative nature is known about the importance of off-diagonal (in band index) contributions to G; however, cases where these corrections seem to be necessary have been extremely rare (but see Chakraborty and Allen[21]). In the present paper all such "band-mixing" effects will be neglected. We will concentrate on including the energy dependence of the band density of states within an isotropic, band-diagonal approximation.

The isotropic average $A(E)$ of a wave-vector-dependent quantity $A(k)$ is defined by

$$A(E) = \sum_k A(k)\hat{\delta}(E-E_k)\ , \tag{3.1}$$

where to simplify notation we have introduced a dimensionless, normalized averaging function given by

$$\hat{\delta}(E-\epsilon) = \delta(E-\epsilon)/N(E)\ .$$

A further approximation necessary to reduce Eq. (2.6) is

$$\sum_{kk'} G(k',i\omega_{n'})B(k,k';i\omega_n - i\omega_{n'})\hat{\delta}(E-E_k)\hat{\delta}(E'-E_{k'}) = G(E',i\omega_{n'})B(E,E';i\omega_n - i\omega_{n'})\ , \tag{3.2}$$

where[22]

$$G(E,i\omega_n)^{-1} \equiv i\omega_n - (E-\zeta)\tau_3 - \Sigma(E,i\omega_n)\ . \tag{3.3}$$

$B(k,k';i\omega_n - i\omega_{n'})$ is any of the three kernels in Eq. (2.6) and $B(E,E';i\omega_n - i\omega_{n'})$ is defined by Eq. (3.2). The self-energy becomes[15(a),15(c)]

$$\Sigma(E,i\omega_n) = T \sum_{|\omega_n'|<\omega_c} \int dE'\tau_3 G(E',i\omega_{n'})\tau_3 N(E')\{\tilde{\lambda}(E,E';i\omega_n - i\omega_{n'}) - \tilde{\mu}^*(E,E') - [\tilde{\Gamma}(E,E')/\pi T]\delta_{nn'}\}\ , \tag{3.4}$$

where

$$\tilde{\lambda}(E,E';i\omega_n)=-\sum_{kk'\nu}|\bar{g}_{kk'\nu}|^2D_\nu(k-k',i\omega_n)\hat{\delta}(E-E_k)\hat{\delta}(E'-E_{k'})\ , \tag{3.5}$$

$$\tilde{\mu}^*(E,E')=\sum_{kk'}\bar{U}(k,k';0)\hat{\delta}(E-E_k)\hat{\delta}(E'-E_{k'})\equiv\bar{U}(E,E';0)\ , \tag{3.6}$$

$$\tilde{\Gamma}(E,E')=\pi n_i\sum_{kk'}|t(k,k';0)|^2\hat{\delta}(E-E_k)\hat{\delta}(E'-E_{k'})\ . \tag{3.7}$$

In the CDOS limit $N(E)\to N(E_F)$, the usual electron-phonon coupling constant λ, pseudopotential μ^*, and impurity width Γ are given by $N(E_F)\tilde{\lambda}(E_F,E_F;0)$, $N(E_F)\tilde{\mu}^*(E_F,E_F)$, and $N(E_F)\tilde{\Gamma}(E_F,E_F)$, respectively. It will become apparent, however, that the normally ubiquitous quantity $N(E_F)$ nowhere appears explicitly in this more general theory, although we will identify in Sec. V an effective average density of states which is useful in an approximate determination of T_c. The Coulomb pseudopotential $\tilde{\mu}^*$ is discussed further in Sec. IV A and in Appendix A.

The E dependence of Σ arises solely from the E dependence of the kernel

$$\tilde{\lambda}_{\text{eff}}(E,E')\equiv\tilde{\lambda}(E,E')-\tilde{\mu}^*(E,E')$$
$$-(1/\pi T)\tilde{\Gamma}(E,E')\ ,$$

which in turn is due to variation with energy of the *character of the wave functions and scattering properties but not the density of states.* In general we expect this variation to be small compared to DOS effects, although this question deserves further study. Information on the E dependence of $\tilde{\lambda}(E,E)$ can be gained by studying the E dependence of the mean-square electron-ion scattering matrix element $I^2(E)$ which enters $\tilde{\lambda}$. Using the calculated electronic structure and wave functions of Klein *et al.*[5] (to be used in the calculations described in Sec. V), it is found that $I^2(E)$ *varies by only 2%* in a 4-mRy region centered at E_F where $N(E)$ changes by a factor of 3. Neglecting this small energy dependence of the kernel gives

$$\Sigma_n=T\sum_{|\omega_n'|<\omega_c}\tilde{\lambda}_{\text{eff}}(i\omega_n-i\omega_{n'})F_{n'}\ , \tag{3.8}$$

where $\Sigma_n\equiv\Sigma(i\omega_n)$, etc, and the density-of-states effects are confined to the factor

$$F_n=\int dE\,\tau_3G(E,i\omega_n)\tau_3N(E)\ . \tag{3.9}$$

Inverting G^{-1} in Eq. (3) leads to

$$\tau_3G(E,i\omega_n)\tau_3=\frac{-i\omega_nZ_n-(E-\zeta+\chi_n)\tau_3}{C(E,i\omega_n)}\ , \tag{3.10}$$

with

$$C(E,i\omega_n)=(E-\zeta+\chi_n)^2+Z_n^2(\omega_n^2+\Delta_n^2)\ . \tag{3.11}$$

The gap function is given by $\Delta_n=\phi_n/Z_n$. Even and odd averages over $N(E)$ result, given by

$$\begin{Bmatrix}N_n\\P_n\end{Bmatrix}=\frac{1}{\pi}\int dE\frac{N(E)}{C(E,i\omega_n)}\times\begin{Bmatrix}Z_n(\omega_n^2+\Delta_n^2)^{1/2}\\E-\zeta+\chi_n\end{Bmatrix}, \tag{3.12}$$

with each average incorporating in the denominator $C(E,i\omega_n)$ an energy shift $\zeta-\chi_n$ and broadening half-width $Z_n(\omega_n^2+\Delta_n^2)^{1/2}$. Both functions are even in ω_n. The following sections describe the effects of a nonconstant $N(E)$ that are included in N_n and P_n, which for a constant density of states reduce to

$$\begin{Bmatrix}N_n\\P_n\end{Bmatrix}\to\begin{Bmatrix}N(E_f)\\0\end{Bmatrix}. \tag{3.13}$$

IV. GENERALIZED ELIASHBERG THEORY

The generalized equations for the Eliashberg self-energies are

$$\omega_nZ_n=\omega_n+\pi T\sum_{m=0}^{N_c}\tilde{\lambda}_{nm}^{(-)}N_me_m+\tilde{\Gamma}N_ne_n\omega_n\ , \tag{4.1}$$

$$\chi_n=-\pi T\sum_{m=0}^{N_c}(\tilde{\lambda}_{nm}^{(+)}-2\tilde{\mu}^*)P_me_m-\tilde{\Gamma}P_ne_n\omega_n\ , \tag{4.2}$$

$$(2n+1)\phi_n=\sum_{m=0}^{N_c}(\tilde{\lambda}_{nm}^{(+)}-2\tilde{\mu}^*)\frac{\omega_n}{\omega_m}N_me_m\phi_m/Z_m$$
$$+\tilde{\Gamma}N_ne_n\phi_n\omega_n/Z_n\ , \tag{4.3}$$

where $\tilde{\lambda}^{(\pm)}$ and the DOS "enhancement" e_n are defined by

$$\widetilde{\lambda}_{nm}^{(\pm)}\equiv\widetilde{\lambda}(i\omega_n-i\omega_m)\pm\widetilde{\lambda}(i\omega_n+i\omega_m)\ , \tag{4.4}$$

$$e_n\equiv\omega_n/(\omega_n^2+\Delta_n^2)^{1/2}\ . \tag{4.5}$$

A nonzero solution to Eq. (4.3) exists only for $T\leq T_c$. However, Eqs. (4.1) and (4.2) may be useful at higher temperatures as well, a fact which is discussed in Sec. VI.

Converting Eq. (4.3) into an equation for the gap function leads to

$$\Delta_n=\pi T\sum_{m=0}^{N_c}\left[(\widetilde{\lambda}_{nm}^{(+)}-2\widetilde{\mu}^*)N_m e_m-\delta_{nm}\sum_{l=0}^{N_c}\widetilde{\lambda}_{nl}^{(-)}N_l e_l\right]\Delta_m/\omega_m\ . \tag{4.6}$$

Explicitly $\widetilde{\lambda}$ is given by

$$\widetilde{\lambda}(i\omega_n-i\omega_m)=2\int d\Omega\,\Omega\widetilde{\alpha}^2F(\Omega)/[\Omega^2+(\omega_n-\omega_m)^2] \tag{4.7}$$

in terms of an *intensive* electron-phonon spectra function (i.e., coupling per electronic state)

$$\widetilde{\alpha}^2F(E,E';\Omega)=\sum_{k,k',\nu}|\bar{g}_{k,k',\nu}|^2\hat{\delta}(E-E_k)\times\hat{\delta}(E'-E_{k'})\times\delta(\Omega-\omega_{k-k',\nu})\ , \tag{4.8}$$

and

$$\widetilde{\alpha}^2F(\Omega)\approx\widetilde{\alpha}^2F(E,E';\Omega)\,|_{E\approx E'\approx E_F}\ .$$

Equations (2.5), (3.12), and (4.1)–(4.3) [or (4.3) replaced by (4.6)] form a system of coupled nonlinear matrix equations which must be solved iteratively for the self-energies at each temperature of interest. Their solution allows (at least in principle) the direct calculation[23] of electronic thermodynamic properties,[15(f)] such as T_c, specific heat, etc. Numerical solutions of these equations have been presented elsewhere[13] (and see below) but a number of effects, and their interpretation, resulting from a complex electronic structure will be discussed in this section. The care which must be exercised in any interpretation of the imaginary frequency equations is exemplified by the "enhancement" e_n defined by Eq. (4.5). Evidently e_n lies in the range $0<|e_n|\leq 1$. The designation "enhancement" is appropriate since, when continued to the real axis, the real part of this function gives the well-known DOS enhancement on the real axis

$$\mathrm{Re}\,e(\omega)=\mathrm{Re}\{\omega/[\omega^2-\Delta^2(\omega)]^{1/2}\}\ . \tag{4.5'}$$

A. The Coulomb pseudopotential

From Eq. (4.2) it follows that the contribution to X from the Coulomb interaction is independent of ω_n. This results in a constant shift X_c in all quasiparticle energies and consequently a compensating shift $\zeta\rightarrow\zeta+X_c$ in the chemical potential. Therefore the Coulomb contribution to X in Eq. (4.2) can be disregarded without loss of generality. On the other hand, phonon and impurity scattering give rise to nonconstant energy shifts X_n which must be retained in an accurate theory.

The pseudopotential $\bar{U}$ in Eq. (3.6) is given as usual[20] as a solution to an integral equation describing the folding-down of high-frequency scattering processes included in $\bar{V}$. The zone-averaged pseudopotential $\widetilde{\mu}^*$ satisfies the approximate relation (see Appendix A)

$$\frac{1}{\widetilde{\mu}^*}=\frac{1}{\widetilde{\mu}}+\bar{N}(\omega_{\mathrm{pl}})\ln\left[\frac{\omega_{\mathrm{pl}}}{\omega_c}\right]\ , \tag{4.9}$$

where $\bar{N}(\omega)$ denotes an average over $N(E)$ on the scale of ω, and $\widetilde{\mu}$ is given in terms of $\bar{V}$ by an equation analogous to (3.6). However, according to the gap equation (4.6) it is approximately the dimensionless quantity $\bar{N}(\omega_\Delta)\widetilde{\mu}^*$ which enters into the determination of the gap function (and hence T_c). Here ω_Δ denotes the range of the average over $N(E)$ appropriate to the gap equation, which will be discussed further below. In the limit of a slowly varying DOS near E_F, $\bar{N}(\omega_\Delta)\rightarrow N(E_F)$ and

$$\frac{1}{\mu^*}=\frac{1}{\mu}+\frac{\bar{N}(\omega_{\mathrm{pl}})}{N(E_F)}\ln\left[\frac{\omega_{\mathrm{pl}}}{\omega_c}\right]\ . \tag{4.10}$$

This leads to a dependence of μ^* upon $N(E_F)$ similar in form to that of Bennemann and Garland,[24] who used $\mu=0.26$ and $\bar{N}(\omega_{\mathrm{pl}})\ln(\omega_{\mathrm{pl}}/\omega_c)=3.85\ (\mathrm{eV\ atom})^{-1}$ for transition metals. However, since μ in Eq. (4.10) is formally proportional to $N(E_F)$, which can vary widely within a given class of metals, Eq. (4.9) is the appropriate relation from which to determine $\widetilde{\mu}^*$. The quantities $\widetilde{\mu}$ and $\bar{N}(\omega_{\mathrm{pl}})$ vary slowly within a class of metals, with the dominant variation arising from scaling with bandwidth.

B. Impurity scattering and "Anderson's theorem"

In the CDOS limit $N_n\rightarrow N(E_F)$, $P_n\rightarrow 0$, X_n vanishes, and the chemical potential is constant.

The gap equation (4.6) reduces to the usual form and, for $\Gamma \equiv N(E_F)\tilde{\Gamma} \rightarrow 0$, the equation (4.1) for Z does likewise. For nonzero Γ the static impurities give a contribution to Z related to disorder broadening of the energy spectrum. Obviously this has no effect on the normal state, since (in the CDOS limit) there is no structure to broaden. The gap-induced structure in the superconducting state, where the quasiparticle DOS is

$$N(E_F)\text{Re}\{\omega/[\omega^2-\Delta^2(\omega)]^{-1/2}\} ,$$

also is unaffected by the broadening since the equations for Z and Δ are uncoupled in this limit. This is a manifestation (indeed, a proof) of Anderson's theorem,[25] which states that superconducting properties (of CDOS systems) are unaffected by dilute nonmagnetic impurities.

The generalized Eliashberg equations above show that this statement of Anderson's theorem breaks down when structure is present in the DOS, due to the disorder broadening of the underlying electronic structure. Although Γ does not enter explicitly into the gap equation (4.6) (due to the energy-conserving nature of this interaction), disorder scattering can lead to important spectral broadening via Z, and conceivably to non-negligible spectral shifts $\chi_n-\zeta$. The effect on the gap and on T_c, is transmitted to the gap equation entirely through the resulting set $\{N_n\}$.

C. $T=T_c$

At $T=T_c$ ($\Delta_n \rightarrow 0$) the alteration of the quasiparticle density of states due to the gap vanishes,

$$\omega_n/(\omega_n^2+\Delta_n^2)^{1/2} \rightarrow \text{sgn}\omega_n ,$$

and the expressions (4.1), (4.2), and (4.6) simplify somewhat. The equation for the (infinitesimal) gap becomes linear and decouples from the remaining equations, which still must be solved iteratively for N_n. The equation determining T_c can be written [Eq. (4.6) with $e_n \rightarrow 1$]

$$\sum_{m=0}^{N_c} \left[\tilde{\lambda}_{nm}^{(+)} - 2\tilde{\mu}^* - \delta_{nm} \left(\frac{2n+1}{N_n} + \sum_{l=0}^{N_c} \tilde{\lambda}_{nl}^{(-)} \frac{N_l}{N_n} \right) \right] N_m \bar{\Delta}_m = 0 , \tag{4.11}$$

where $\bar{\Delta}_m = \Delta_m/\omega_m$. Written in this form the T_c equation is a straightforward generalization of the CDOS expression, as given for example by Allen and Dynes.[26] Ignoring for the moment corrections to the kernel diagonal, the primary change is the replacement of the CDOS eigenvector $\bar{\Delta}_n$ by $N_n\bar{\Delta}_n$. This replacement has no effect upon either T_c or the eigenvector, whose components are now $N_n\bar{\Delta}_n$. This means that (at this level of approximation) Δ_n will be altered by DOS structure in proportion to N_n^{-1}. A similar correction to the gap occurs at $T<T_c$, and this indicates that the analytic continuation $\Delta(\omega)$ can be altered substantially[13,27] by energy dependence of the DOS.

The correction due to DOS structure to the phonon contribution to Z_n-1, proportional to N_l in Eq. (4.11), *tends* to be canceled by N_n, while the factor N_n^{-1} multiplying $(2n+1)$ in the diagonal can be regarded as the self-consistent response of Δ_n to the DOS structure. It is this latter effect which gives rise to much of the correction to T_c compared to the CDOS limit. The structure of Eq. (4.11) will be clarified further in Sec. V where an approximate T_c equation is discussed.

V. DISCUSSION AND CALCULATIONAL RESULTS AT LOW TEMPERATURE

A. How much DOS variation?

The system of generalized Eliashberg equations has been applied to Nb_3Sn and Nb at $T=T_c$. Technical aspects of the numerical solution are discussed in Appendix B. For Nb_3Sn the corrections to the CDOS results are substantial, both for T_c and for the self-energies Δ_n, $\omega_n Z_n$, and χ_n. Crystalline Nb was checked as a possible fringe case, where corrections might be noticeable if not really important. The DOS of Nb is characterized by a large value of $N(E_F) \cong 10$ (Ry spin)$^{-1}$ with E_F lying 20 mRy above a peak, and the energy variation being described sufficiently well by a slope of -200 (Ry^2 spin)$^{-1}$ over a range of ± 20 mRy $= \pm 3 \times 10^3$ K around E_F. The correction to T_c was found to be 0.4% (downward), with correspondingly small corrections to the self-energies at T_c. Although this correction is well below the absolute accuracy of the Eliashberg equations as derived (keeping only certain classes of diagrams) and applied (especially the treatment of the Coulomb interaction), it nevertheless represents faithfully the accuracy of the CDOS approximation in Nb and in metals with similar or less DOS structure near E_F. A preliminary report of the Nb_3Sn calculations has been reported[13] and further results are discussed below.

B. Approximate relations for T_c

In the CDOS limit T_c is determined by α^2F and μ^*, or equivalently,

$$T_c = T_c[\lambda, g(\omega), \mu^*] \;, \tag{5.1}$$

where α^2F is described by a strength λ and shape function

$$g(\omega) = (2/\lambda\omega)\alpha^2F(\omega) \;.$$

Generalizing the pioneering work of McMillan,[28] Allen and Dynes[26] showed that, for widely varying strengths and shape functions, this *functional* of g can be replaced to high accuracy by a *function* involving only two moments $\omega_{\log}$ and ω_2 of g.

$$T_c \approx T_c^{\mathrm{AD}}(\lambda, \omega_{\log}, \omega_2, \mu^*) \;. \tag{5.2}$$

One of the most useful applications of such an approximate T_c equation is the extraction of λ from experimental data on T_c and reasonable estimates[29] of $\omega_{\log}$, ω_2, and μ^*.

In the previous sections it has been shown that the general functional form of T_c is

$$T_c = T_c[\tilde{\lambda}, \tilde{g}(\omega), \tilde{\mu}^*; N(E), \tilde{\Gamma}] \;, \tag{5.3}$$

where $\tilde{g}$ is defined analogously to g. The form of the gap equation (4.6), together with the work of Allen and Dynes, suggests an approximate T_c equation of the form

$$T_c = T_c(\tilde{\lambda}, \omega_{\log}, \omega_2, \tilde{\mu}^*; N_\lambda, N_\mu, N_\Delta, \tilde{\Gamma}) \;, \tag{5.4}$$

where N_λ, N_μ, and N_Δ are averages over $N(E)$. A few general features of these averages will be noted here.

The average denoted N_λ is that which should multiply $\tilde{\lambda}^{(-)}$ in the kernel diagonal in the approximation

$$\sum_{l=0}^{N_c} \tilde{\lambda}_{nl}^{(-)} N_l \rightarrow N_\lambda \sum_{l=0}^{N_c} \tilde{\lambda}_{nl}^{(-)} \;. \tag{5.5}$$

Since $\tilde{\lambda}$ decreases as ω_m^{-2} for $\omega_m \gg \bar{\Omega}$, N_λ will correspond approximately to a Lorentzian average of $N(E)$ over a frequency half-width $\bar{\Omega}$ around E_F (actually ζ).

In the off-diagonal terms the corresponding replacement is

$$\sum_{m=0}^{N_c} \tilde{\lambda}_{nm}^{(+)} N_m \bar{\Delta}_m \rightarrow N_\Delta \sum_{m=0}^{N_c} \tilde{\lambda}_{nm}^{(+)} \bar{\Delta}_m \;. \tag{5.6}$$

However, since $\bar{\Delta}_m$ decreases rapidly with increasing ω_m, even changing sign for $\omega_m \lesssim \bar{\Omega}$, N_Δ averages over a smaller region than does N_λ, for example, on the order of $\bar{\Omega}/2$.

The average N_μ multiplying $\tilde{\mu}^*$ is less straightforward, since $\tilde{\mu}^*$ has no frequency cutoff to make a partial sum coverage. Numerical solutions[30,31] show that Δ_n approaches a negative constant value Δ_∞ for large n (for nonvanishing $\tilde{\mu}^*$). Obviously N_n also approaches a constant average DOS value N_∞. If both N_n and Δ_n have approached their asymptotic value at $n = k < N_c$, it follows that N_μ, given by

$$N_\mu \equiv \sum_0^{N_c} N_n \bar{\Delta}_n \Big/ \sum_0^{N_c} \bar{\Delta}_n$$

$$\cong \frac{\sum_0^{k-1} N_n \bar{\Delta}_n + \frac{1}{2} N_\infty \Delta_\infty \ln(N_c/k)}{\sum_0^{k-1} \bar{\Delta}_n + \frac{1}{2} \Delta_\infty \ln(N_c/k)} \;, \tag{5.7}$$

is weakly dependent on the cutoff N_c. This cutoff dependence is artificial and arises from the inconsistent treatment given to $\tilde{\mu}^*$ in folding $\tilde{\mu}$ down to $\tilde{\mu}^*$. The energy integral leading to Eq. (4.9) does not take into account the full variation of $N(E)$ whereas the "unfolding" to the cutoff N_c in Eq. (5.7) is taking this energy dependence into account. It is straightforward to correct this discrepancy by generalizing Eq. (4.9), that is, by using the relation (A5). However, the following approximation will suffice to illustrate some effects of DOS structure.

Owing to the rapid decrease of Δ_n with n and the $(2n+1)^{-1}$ factor in $\bar{\Delta}_n$, the DOS average,

$$N_\mu(M) \equiv \sum_{n=0}^{M} N_n \bar{\Delta}_n \Big/ \sum_{n=0}^{M} \bar{\Delta}_n \;, \tag{5.7$'$}$$

for small M "converges" (i.e., becomes stationary with respect to M) rapidly before the cutoff dependence mentioned above becomes a consideration and leads to the unwanted limit $N_\mu \rightarrow N_\infty$. In a preliminary report[13] of this work applied to Nb$_3$Sn (also see below) the first term alone

$$N_\mu(M=0) = \bar{N}(\pi T_c Z_0) \equiv N_{\mathrm{eff}}$$

was used in the CDOS theory, giving an approximate value T_c^{eff} which could be compared to numerical solutions of the full system of matrix equations for T_c. In essence T_c^{eff} is given by (for $\tilde{\Gamma}=0$)

$$T_c^{\mathrm{eff}} = T_c^{\mathrm{AD}}(N_{\mathrm{eff}}\tilde{\lambda}, \omega_{\log}, \omega_2, N_{\mathrm{eff}}\tilde{\mu}^*) \tag{5.8}$$

(although numerical solutions to the CDOS equations were actually used rather than the Allen-Dynes equation). Note that

$$\pi T_c Z_0 \approx 0.85 - 0.90\omega_2 \approx \bar{\Omega}/2$$

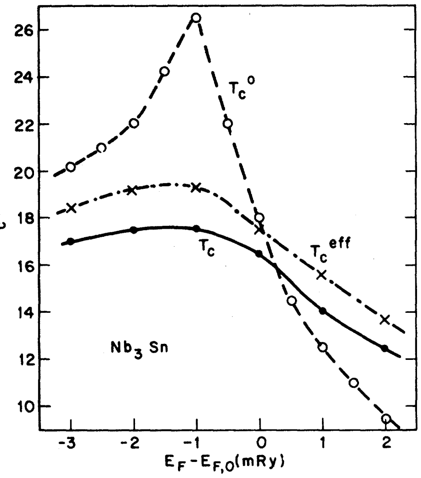

FIG. 2. Superconducting transition temperature T_c of Nb_3Sn vs Fermi-level position, calculated within different approximations. Full line, solution from full energy-dependent equations; dashed line, solution assuming CDOS $N(E)=N(E_F)$; dot-dash line, solution assuming CDOS $N(E)=N_{eff}$ (see text).

for Nb_3Sn ($T_c=18$ K, $Z_0=2.7$, $\omega_2=175$ K). The results of this approximation are shown in Fig. 2, where it is evident that T_c^{eff} reflects the trends of the numerical solution quite well as the assumed value of E_F is varied, although being ~1.5 K too large. The crude approximation T_c^0 resulting from the assumption $N(E)=N(E_F)$ is seen in Fig. 2 to give a much stronger $N(E_F)$ dependence than actually occurs.

For nonzero impurity scattering each DOS average N_n has its broadening half-width $\omega_n Z_n$ increased by $\tilde{\Gamma} N_n$ [see Eq. (4.1)]. A low-order approximation can include this by increasing by $\Gamma_{eff} \equiv N_\lambda \tilde{\Gamma}$ each of the widths which determine N_λ, N_Δ, and N_μ, of which the former must be calculated self-consistently (at least in principle). The calculations described below result from numerical solutions to the full energy-dependent equations, however.

The quantities N_λ, N_Δ, and N_μ offer a reasonable possibility of obtaining a realistic value of T_c without solving nonlinear coupled matrix equations. Unfortunately it is a monumental task to ascertain even an appropriate form of the approximate T_c equation envisioned in Eq. (5.4), as this would involve full solutions for a wide variety of shapes of $N(E)$ and $\tilde{g}(\omega)$ as well as coupling strengths $\tilde{\lambda}$, $\tilde{\mu}^*$, and $\tilde{\Gamma}$. Worse, it begins to appear hopeless to extract unambiguous information from an experimental value of T_c in the face of so many unknown parameters. The only compensation is that the behavior of T_c with the level of imperfection [$T_c(\tilde{\Gamma})$] can be incorporated into the analysis. A more realistic approach for interpreting experimental data is to use a single average N_{eff}, with $N_{eff}=N_\lambda$ being a good choice, in the CDOS expression of Allen and Dynes. This in effect is the usual practice, except that the value of $\lambda_{eff}=N_{eff}\tilde{\lambda}$ extracted in this manner may differ from the mass enhancement value derived from heat capacity or other measurements.

Although the DOS average appropriate for an approximate T_c equation given above differs in detail from that of Nettel and Thomas,[9] the spirit of the approximation is similar to theirs. The more rigorous, but linear, approach of Lie and Carbotte[11] for calculating $\delta T_c/\delta N(E)$ follows from the present formulation by calculating the correction ΔT_c arising from an infinitesimal variation of energy E from a constant DOS given by

$$\Delta N(E')=\epsilon\delta(E'-E) .$$

It could be of interest to study the effects of the supralinear terms for a particular DOS function using the present theory. However, the Lie-Carbotte results provide an important intuitive grasp of the general behavior of $\delta T_c/\delta N(E)$ as well as a first approximation for numerical calculations.

C. Defect dependence of T_c and $N(E_F)$

It was observed in Sec. V B that experimental data on $T_c[\tilde{\Gamma}]$ [i.e., T_c versus defect concentration n_i, since $\tilde{\Gamma}=\pi n_i \mid t^2 \mid$ from Eq. (3.7)] provide

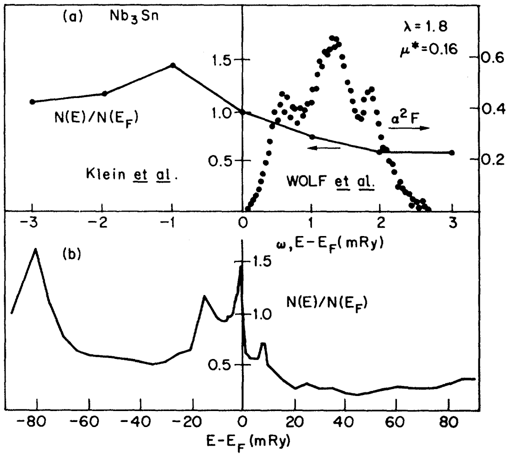

FIG. 3. Comparison of electron and phonon energy scales for Nb_3Sn. (a) $\alpha^2F(\omega)$ from tunneling data by Wolf *et al.* (Ref. 32) and $N(E)$ function calculated by Klein *et al.* (Ref. 5), shown on the same mRy scale. (b) Same $N(E)$ function on a scale of ~1 eV.

direct information on the energy variation of $N(E)$. Calculation of $T_c(\tilde{\Gamma})$ has been carried out for Nb$_3$Sn using the DOS function calculated by Klein *et al.*[5] For $\tilde{\alpha}^2F$ we have assumed

$$\alpha^2F(\omega)=\bar{N}(\omega_{\text{ph}})\tilde{\alpha}^2F(\omega)\ , \tag{5.9}$$

$\omega_{\text{ph}}=300$ K, with $\alpha^2F(\omega)$ derived from tunneling data by Wolf *et al.*[32] Both $N(E)$ and α^2F are shown in Fig. 3 on the same scale to allow an easy comparison of their energy variations. For $\tilde{\mu}^*$ the value $\mu^*=0.16$ determined by Wolf *et al.* has been used in the form $N(E_F)\tilde{\mu}=0.16$.

To compare with experimental data the defect-broadening half-width Γ was related to the residual resistivity ρ_0 by

$$\rho_0=4\pi\Gamma/\Omega_p^2\ , \tag{5.10}$$

$$\Omega_p^2=(4\pi e^2/3)N(E_F)v_F^2\ , \tag{5.11}$$

with[33] $\hbar\Omega_p=4.0$ eV. The experimental data on $\rho(T_c)\approx\rho(0)$ has been converted to the "true" residual resitivity ρ_0 by the use of the parallel resistor formula

$$\frac{1}{\rho(0)}=\frac{1}{\rho_0}+\frac{1}{\rho_{\max}}\ , \tag{5.12}$$

$\rho_{\max}=150\ \mu\Omega$ cm, since Weismann *et al.*[34] have found that ρ_0 given by this expression, and not $\rho(0)$, is approximately linear with damage-inducing radiation dose. The theoretical prediction is compared to four sets[35] of experimental data in Fig. 4. The calculation is consistent with experimental data for residual resistivities below 75 $\mu\Omega$ cm. For larger disorder the theoretical prediction approaches the asymptotic limit $T_c\simeq 9$ K whereas the experimental values saturate at $T_c\simeq 3$ K. This indicates that, for $\rho_0>75\ \mu\Omega$ cm, the disorder is decreasing the electron-phonon coupling $\tilde{\alpha}^2(\omega)$ and/or hardening the phonon spectrum $F(\omega)$, neither of which is included in the present theory which treats α^2F as independent of disorder.

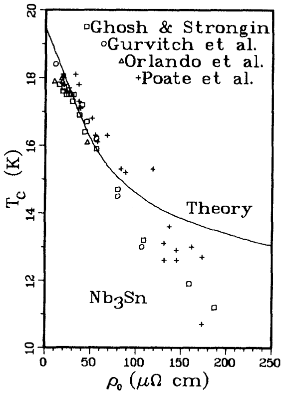

FIG. 4. Calculated T_c of Nb$_3$Sn (full curve) vs "true" residual resistivity ρ_0 (i.e., from parallel resistor formula) compared with experimental data (Ref. 35). The theory is not expected to be accurate for large defect concentration ($\rho_0>75\ \mu\Omega$ cm) since changes in $\tilde{\alpha}^2F$ are not included in the theory.

The correspondence between defect concentration and residual resistivity ($\tilde{\Gamma}\leftrightarrow\rho_0$) is not as simple as Eq. (5.10) implies. It should be observed, for example, that Γ in Eq. (5.10) must be determined self-consistently from the relation

$$\Gamma=\bar{N}(\Gamma)\tilde{\Gamma}\ , \tag{5.13}$$

where, as will be shown below, the Γ dependence of $\bar{N}(\Gamma)$ is strong. Therefore, although $\tilde{\Gamma}$ increases linearly with disorder, Γ is distinctly sublinear. However, the factor Ω_p^2 in a suitably generalized version of Eq. (5.10) also contains the factor $\bar{N}(\Gamma)$ so the DOS dependence of ρ_0 cancels. As a result the defect concentration dependence of ρ_0 *goes inversely with that of* v_F^2, a result analogous to an equivalent observation for the phonon-limited resistivity made previously by Allen.[36] This result can be written

$$\rho_0=3\tilde{\Gamma}/e^2v_F^2[\Gamma(\tilde{\Gamma})]\ . \tag{5.14}$$

We find by calculation, however, that $v_F^2(\Gamma)\propto 1/\bar{N}(\Gamma)$ [since $\bar{\Omega}_p^2(\Gamma)$ is constant to within 2%], which makes Eq. (5.14) *numerically* equivalent to

$$\rho_0\leftrightarrow[4\pi/\Omega_p^2(E_F)]\bar{N}(\Gamma)\tilde{\Gamma}\ . \tag{5.14$'$}$$

Conceptually Eqs. (5.14) and (5.14′) *are not at all equivalent* and the former relation gives the correct physical picture.

In Fig. 5 the effective defect broadening (or

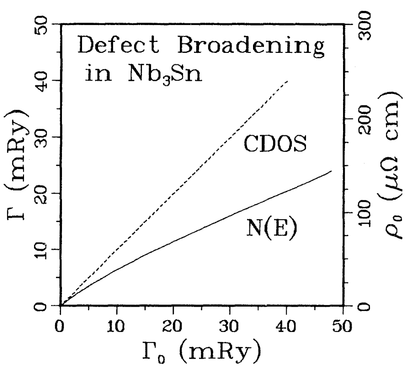

FIG. 5. Self-consistently determined defect broadening width Γ (equivalently residual resistivity ρ_0)—full line—vs disorder Γ_0, determined from $N(E)$ shown in Fig. 3. The dashed line gives the CDOS approximation $\Gamma=\Gamma_0$.

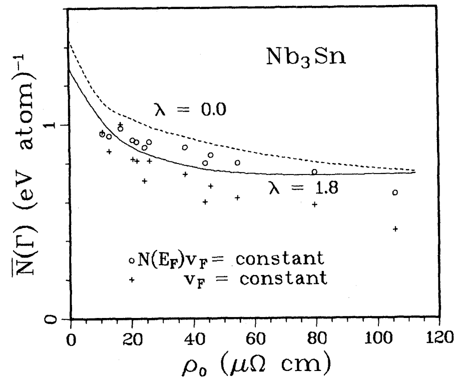

FIG. 6. Effective density of states $\overline{N}(\Gamma)$ vs residual resistivity ρ_0 for Nb_3Sn. Solid line: theory, including *e*-ph interaction with $\lambda=1.8$. Dashed line: theory, no *e*-ph interaction. Symbols: experimentally inferred values (Ref. 38), assumed two different constraints on $N(E_F)v_F$ with varying disorder.

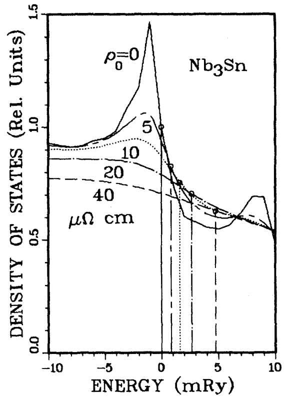

FIG. 7. Effect of defect broadening on the $N(E)$ function shown in Fig. 3. Vertical lines indicate the respective Fermi levels, determined from conservation of electrons. Circles denote $\overline{N}(\Gamma)=N(E_F)$. The best samples of Nb_3Sn have residual resistivities $\rho_0\approx 10$ $\mu\Omega$ cm, which precludes extreme energy variation of the density of states.

equivalently, ρ_0) is plotted versus

$$\Gamma_0=N(E_F)\tilde{\Gamma}=\pi n_i N(E_F)\,|\,t^2\,|\ .$$

Owing to broadening of the peak in $N(E)$ near E_F, Γ increases more slowly than that for a CDOS $N(E)\equiv N(E_F)$, shown by the dashed line. However, for $\rho_0\geq 50$ $\mu\Omega$ cm, Γ is *approximately* linear with defect concentration, just as the data of Weismann *et al.*[34] for ρ_0 are approximately linear with radiation fluence in this range.

The behavior of the factor of $N(E_F)$ in the linear specific-heat coefficient γ versus residual resistivity may provide more direct information on $N(E)$ than does $T_c(\rho_0)$, since only a straightforward Lorentzian broadening[37] of $N(E)$ is involved. In the few cases which have been studied systematically, however, γ has been inferred instead from the temperature dependence of the upper critical magnetic field,[38] which involves independent information (or assumptions) about the values of material constants such as λ, v_F, mean free path l, etc., as well as an assumption about the behavior of band-structure-related quantities with defect concentration. The resulting values of $\overline{N}(\Gamma)$ for Nb_3Sn obtained by Ghosh *et al.*,[38] resulting from the assumption that $N(E_F)v_F$, or secondly, v_F itself, remains constant with increasing disorder, are compared in Fig. 6 with that calculated from the DOS function in Fig. 3. Calculated values of $\overline{N}(\Gamma)$ are shown both for the (usually assumed) case where only defect broadening is taken into account (dashed line), and the more general case in which *e*-ph broadening is included (full line).

The calculated values including *e*-ph broadening are in slightly better agreement with the empirical values obtained assuming $N(E_F)v_F=\text{const}$ [however, the argument given above in the discussion of $T_c(\rho_0)$ indicates $N(E_F)v_F^2)=\text{const}$ would be the proper assumption]. The analysis of Ghosh *et al.* of course also needs generalizing along the lines of the present theory. It is clear from Fig. 6 that extrapolation from the existing data to obtain a "perfect crystal value" of $N(E_F)$ may not be valid, since a kink may occur at or below 10 $\mu\Omega$ cm. The degree of broadening of the full $N(E)$ curve is illustrated more clearly in Fig. 7. A peak of width 3–4 mRy or less is virtually lost for a residual resistivity of 10 $\mu\Omega$ cm, which corresponds to the highest quality samples of Nb_3Sn. Such a large perfect-crystal value of $N(E_F)$ implies a tendency toward defect formation, which serves to lower $N(E_F)$ and thereby decreases the number of electrons at high energy, resulting in a more stable material.

D. Defect dependence of T_c: Previous studies

There have been several previous applications of broadening to account for properties, especially T_c, of *A*15 compounds. Most of these have been phenomenological, as typified particularly by the work of Mattheiss and Testardi.[39,40] The studies of Aleksandrov, Elesin, and Kazeko,[41] and Huang, Chu, and Ting,[41] however, have used a more fundamental approach. Both groups studied T_c using a weak-coupling formalism and model DOS functions to illustrate the effect of defect broadening of $N(E)$ upon T_c.

Aleksandrov *et al.*[41] purported to explain the saturation in Nb_3Sn of T_c at 3 K for high defect concentration solely in terms of DOS broadening. The present generalized theory and realistic DOS function shows saturation at $\sim 8-9$ K if only defect broadening is taken into account. In addition, this limit depends on the DOS function on only a large (~ 1 eV) scale, for which all band-structure calculations[4,5] give results similar (*modulo* $5-10\%$ bandwidth-type differences arisings from different exchange-correlation approximations, etc.) to those of Klein *et al.*[5] which were used here. A similar limit (~ 7 K) follows from the DOS broadening study of Soukoulis and Papaconstantopoulos,[42] if $T_c(10\ \mu\Omega\,\text{cm})$ is normalized to the experimental value of 18.6 K. To understand the 3-K saturation it is necessary to invoke a weakening in the strength of $\tilde{\alpha}^2F$ by approximately a factor of 2. This weakening may result from weaker coupling or harder phonons. In fact, both of these effects have recently been observed in tunneling studies of Nb_3Al (Ref. 43) and Nb_3Ge (Ref. 44) with varying degrees of disorder.

Huang *et al.*[41] assumed a singular one-dimensional DOS and obtained results similar to those of Aleksandrov *et al.* and the present results. They concluded that, due to DOS variation near E_F, a high T_c compound can have a small value of $N(E_F)$. A look at Fig. 7 shows that this cannot be the case for *A* 15 compounds with appreciable amounts of disorder, as in all samples of Nb_3Ge, Nb_3Al, or for that matter, Nb_3Sn. For $\rho_0 = 10$ $\mu\Omega\,\text{cm}$, i.e., a clean Nb_3Sn sample, the broadening half-width Γ is 1.6 mRy=250 K, which is roughly equal to the maximum phonon frequency Ω. Thus $\bar{N}(\Omega)$, which determines T_c (see Sec. V B), cannot be much different from the value of $N(E)$ at E_F [$\bar{N}(\Gamma)$ in the present notation]. A *very low* ρ_0, high-T_c crystal may have a relatively low value of $N(E_F)$ if a large peak lies within $\sim\Omega$ of E_F, however.

Other mechanisms involving defect broadening have been proposed to account for the degradation of T_c by defects. Meisel and Cote[45] suggested that an assumed inability of phonons with wavelength longer than the electron mean free path to scatter electrons effectively (and hence bind Cooper pairs) could account for the defect dependence of high T_c compounds. This cannot explain the *increase* in T_c with ρ_0 in low-T_c materials,[46] however. Moreover, if this "phonon-ineffectiveness" concept is accepted it is very difficult to understand the rather large T_c and measured α^2F of highly disordered Mo (Kimhi and Geballe, Ref. 46). Ruvalds and Soukoulis[47] have attributed most of the high T_c (at least in Nb_3Ge and V_3Si) to an acoustic plasmon mechanism which decreases in strength as the electronic spectrum is broadened. However, there is strong evidence from tunneling measurements that the electron-phonon interaction itself is strong enough to account for the high T_c in V_3Ga (Ref. 48), Nb_3Sn (Ref. 32), Nb_3Al (Ref. 43), and Nb_3Ge (Ref. 44), so there is now little reason to except the acoustic plasmon mechanism to apply to any *A* 15 compounds.

VI. NORMAL-STATE SPIN SUSCEPTIBILITY

In Sec. IV it was shown that in general T_c does not provide a measure of $N(E_F)$, but rather of an average of the DOS over a region $\pi T_c Z_0$ or larger. In this section we investigate what information about $N(E)$ is contained in the spin susceptibility χ_{sp}. For the sake of generality the full k dependence of the expressions will be retained as far as possible.

A. General considerations

The magnetization M is given by the difference in number of spin-up and spin-down electrons times the moment per electron,

$$M(\zeta,T)=\mu_B(N_{e,\uparrow}-N_{e,\downarrow}) = \mu_B\sum_\sigma \sigma N_{e,\sigma}\ , \tag{6.1}$$

with

$$N_{e,\sigma}=T\sum_{k,n} G_\sigma(k,i\omega_n)e^{i\omega_n\epsilon} \tag{6.2}$$

and

$$G_\sigma^{-1}(k,i\omega_n)=i\omega_n-(E_k-\zeta-\mu_B\sigma H) -\Sigma_\sigma(k,i\omega_n)\ , \tag{6.3}$$

where H is the magnetic field. Luttinger[49] has shown how this "self-evident" *exact* expression for M can be derived diagrammatically.

The measured zero-field susceptibility is given by

$$\chi_{\text{sp}}=\left(\frac{\partial M}{\partial H}\right)_{T,N_e}\Bigg|_{H=0}=\left(\frac{\partial M}{\partial H}\right)_{T,\zeta}\Bigg|_{H=0,\zeta=\zeta(N_e)}$$

$$=\mu_B^2T\sum_{k,n,\sigma}\sigma^2G_\sigma^2(k,i\omega_n)e^{i\omega_n\epsilon}\left(-\frac{dG_\sigma^{-1}(k,i\omega_n)}{d(\mu_B\sigma H)}\right)_{H=0} \tag{6.4}$$

$$=-2\mu_B^2T\sum_{k,n}G^2(k,i\omega_n)[1+\Sigma'(k,i\omega_n)]\ , \tag{6.5}$$

where we have used Eq. (6.3) and the expansion

$$\Sigma_\sigma(k,i\omega_n)=\Sigma(k,i\omega_n)-\mu_B\sigma H\Sigma'(k,i\omega_n)+O(H^2)\ . \tag{6.6}$$

Equation (6.5) is an *exact* expression for χ_{sp} in terms of the renormalized Green's function and the field derivative of the self-energy. As can be seen from Wolff's[50] diagrammatic theory for χ_{sp}, the G^2 term in Eq. (6.5) arises from the simple, but renormalized, bubble diagram in Fig. 8(a), whereas the $G^2\Sigma'$ term arises from all vertex corrections (i.e., diagrams with other than self-energy insertions to G). With Σ given by the diagrams of Fig. 1, we can write, introducing $J_\sigma=-dG_\sigma^{-1}/d(\mu_B\sigma H)\,|_{H=0}=J_{-\sigma}=J$,

$$J(k,i\omega_n)=1-\frac{d}{d(\mu_B\sigma H)}T\sum_{k'n'}\tilde{\lambda}_{\text{eff}}(k,k';i\omega_n-i\omega_n)G_\sigma(k',i\omega_{n'}) \tag{6.7}$$

$$=1+T\sum_{k'n'}\tilde{\lambda}_{\text{eff}}(k,k';i\omega_n-i\omega_{n'})G^2(k',i\omega_{n'})J(k',i\omega_{n'})$$

$$-T\sum_{k'n'}\left(\frac{d}{d(\mu_B\sigma H)}\tilde{\lambda}_{\text{eff}}(k,k';i\omega_n-i\omega_{n'})\right)_{H=0}G(k',i\omega_{n'})\ . \tag{6.7$'$}$$

The second term in Eq. (6.7′) describes "ladder-type" vertex corrections (see below), with a typical graph shown in Fig. 8(b). The third term represents field corrections to the effective electron-electron interaction, with the lowest-order phonon contribution shown in Fig. 8(c). There is of course a large class of diagrams for χ_{sp} which are not included in Eq. (6.7) by virtue of the approximation for Σ from which this equation is derived.

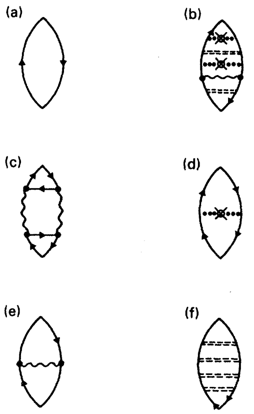

FIG. 8. Susceptibility diagrams discussed in the text. For simplicity the *renormalized Green's function is denoted by single full lines* rather than double lines as in Fig. 1. Other notation is as in Fig. 1.

For $T\rightarrow0$ Luttinger[49] has shown that, as long as $\gamma(\omega)$ $[\Sigma(\omega)\equiv m(\omega)-i\gamma(\omega)]$ vanishes as fast as ω^2 as $\omega\rightarrow0$, M is given by

$$M=\mu_B\sum_{k\sigma}\sigma\Theta(\zeta-\mathscr{E}_{k\sigma}) \tag{6.8}$$

where Θ is the unit step function and $\mathscr{E}_{k\sigma}$ is the renormalized energy given by

$$\mathscr{E}_{k\sigma}=E_{k\sigma}-m_\sigma(k,\mathscr{E}_{k\sigma}-\zeta)\ . \tag{6.9}$$

The susceptibility is given by

$$\chi_{\text{sp}}(T=0)=2\mu_B\sum_{k\sigma}\left(-\frac{d\mathscr{E}_{k\sigma}}{dH}\right)\delta(\zeta-\mathscr{E}_{k\sigma})\ . \tag{6.10}$$

The derivatives

$$\vec{\nabla}_k\mathscr{E}_{k\sigma}=\vec{\nabla}_kE_{k\sigma}-\vec{\partial}_km_\sigma(k,\mathscr{E}_{k\sigma}-\zeta)$$

$$-\partial_\omega m(k,\omega)\,|_{\omega=\mathscr{E}_{k\sigma}-\zeta}\vec{\nabla}_k\mathscr{E}_{k\sigma}\ , \tag{6.11}$$

$$\frac{d\mathscr{E}_{k\sigma}}{dH}=\frac{dE_{k\sigma}}{dH}-\frac{\partial}{\partial H}m_\sigma(k,\mathscr{E}_{k\sigma}-\zeta)$$
$$-\partial_\omega m(k,\omega)\,|_{\omega=\mathscr{E}_{k\sigma}-\zeta}\frac{d\mathscr{E}_{k\sigma}}{dH}\ , \tag{6.12}$$

at the Fermi surface $\mathscr{E}_{k\sigma}=\zeta$ become

$$\vec{\nabla}_k\mathscr{E}_{k\sigma}=[\vec{\mathrm{v}}_k-\vec{\partial}_k m_\sigma(k,0)]/(1+\lambda_k)\ , \tag{6.13}$$

$$\frac{d\mathscr{E}_{k\sigma}}{dH}=-\mu_B\left[\sigma+\frac{\partial m_\sigma(k,0)}{\partial(\mu_B H)}\right]\Big/(1+\lambda_k)\ , \tag{6.14}$$

where $\lambda_k=-\partial_\omega m(k,\omega)\,|_{\omega=0}$ is the usual mass renormalization. Equation (6.10) becomes

$$\chi_{\mathrm{sp}}(T=0)=2\mu_B^2 N(\zeta)\left\langle\left[1+\frac{\partial m_\uparrow(k,0)}{\partial(\mu_B H)}\right]\Big/\,|\,\hat{v}_k-\vec{\nabla}_k m(k,0)/v_k\,|\right\rangle . \tag{6.15}$$

Here $v_k=|\,\vec{\mathrm{v}}_k\,|$ and $\vec{\mathrm{v}}_k=v_k\hat{v}_k$, and the angle brackets $\langle\ \rangle$ denote a Fermi-surface average.

Equation (6.10) expresses χ_{sp} in terms of a renormalized density of states, including mass enhancement from Eq. (6.9), and a susceptibility per state $-d\mathscr{E}_{k\sigma}/dH$ which also includes a mass enhancement factor [Eq. (6.14)]. Equation (6.15) expresses χ_{sp} in terms of the bare factor $N(\zeta)$ in which the total mass enhancement cancels out. That the phonon mass enhancement cancels out was first recognized by Quinn and Ferrell,[51] who interpreted the cancellation as the result of each of the spin-split bands carrying its own mass renormalization with it rigidly.

Reverting to the isotropic approximation for G, the relation for the thermal distribution function

$$f(E-\zeta)=T\sum_n G(E,i\omega_n)e^{i\omega_n\epsilon} \tag{6.16}$$

can be differentiated to yield

$$-\frac{df(E-\zeta)}{dE}=-T\sum_n G^2(E,i\omega_n)\ , \tag{6.17}$$

the convergence factor being unnecessary here. Equation (6.5) for χ_{sp} can therefore be written

$$\chi_p(T)=2\mu_B^2\int dE\left[-\frac{df(E-\zeta)}{dE}\right]$$
$$\times N(E)[1+\Sigma'(E,T)]\ , \tag{6.18}$$

with $\Sigma'(E,T)$ being defined from Eq. (6.5) by this equation.

The crucial feature of this expression is that interactions can alter $f(E)$ drastically from its free-particle counterpart

$$f_0(E)=[\exp(E/T)+1]^{-1}\ .$$

The behavior of f has been presented elsewhere[52] for the case of electrons interacting with an Einstein phonon spectrum of strength λ, where it was found that, with increasing λ, $-df/dE$ becomes ever more long ranged, resulting in considerably increased averaging over $N(E)$ as well as a greater variation of $\zeta(T)$ given by the isotropic form of Eq. (6.2):

$$N_e=2\int dE\,f(E-\zeta)N(E)\ . \tag{6.2$'$}$$

For even moderate values of λ, of the order of 0.5, f differs significantly from f_0 and results in an enhanced temperature dependence of χ_{sp} in Eq. (6.18). Bhatt[53] has found previously that a low-temperature expression leads to an enhancement $(1+\lambda)$ of the T dependence of χ_{sp}.

Returning to the expression (6.7) for the enhancement J, neglect of the field dependence of the interaction leads to

$$J(i\omega_n)=1+T\sum_{n'}\tilde{\lambda}_{\mathrm{eff}}(i\omega_n-i\omega_{n'})$$
$$\times\int dE\,N(E)G^2(E,i\omega_{n'})J(i\omega_{n'}) \tag{6.19}$$

in the isotropic approximation. As was the case for the self-energy in Sec. III, the (assumed) independence of $\tilde{\lambda}_{\mathrm{eff}}$ on E_k and $E_{k'}$ leads to an E-independent J. Also as was found for Σ, the distinct frequency dependences of the Coulomb, phonon, and defect interactions lead to different characteristic behaviors for J.

B. Coulomb interaction

In the presence of only Coulomb interactions (in the approximation of Secs. II and III) f is essentially unchanged from f_0. In the range of interest in Eq. (6.18), of the order of πT, the frequency dependence of the screened exchange interaction, which will be denoted as usual by I, can be neglected. Equation (6.19) becomes ($J_\uparrow = J_\downarrow = J$)

$$J = 1 + I \int dE \left[-\frac{df(E-\zeta)}{dE} \right] N(E) J$$

$$= 1/[1 - IN_{\text{eff}}(\zeta)] \; , \tag{6.20}$$

where

$$N_{\text{eff}}(\zeta) = \int dE \left[-\frac{df(E-\zeta)}{dE} \right] N(E) \tag{6.21}$$

is the effective density of states at ζ at temperature T. With the enhancement $J = 1 + \Sigma'$ given in Eq. (6.20), Eq. (6.18) becomes the usual Stoner-enhanced expression for χ_{sp}.

C. Interaction with defects

Defects drastically alter the occupation of *crystalline* eigenstates, even at $T=0$. Assuming a constant density of states, it is straightforward to show that f is given (in the dilute limit) by the convolution of f_0 with a Lorentzian of width $\Gamma = N(E_F)\tilde{\Gamma}$:

$$f(E) = \int dE' f_0(E') \frac{(\Gamma/\pi)}{(E-E')^2 + \Gamma^2} \; . \tag{6.22}$$

If $N(E)$ varies on the scale of $N(E_F)\tilde{\Gamma}$, Γ must be determined self-consistently as discussed in Sec. V C.

Defects give rise to a susceptibility enhancement given by

$$J(i\omega_n) = 1 + (\tilde{\Gamma}/\pi) \int dE\, N(E) G^2(E, i\omega_n) J(i\omega_n) = 1/[1 - \bar{I}_i(i\omega_n)] \; , \tag{6.23}$$

where $\bar{I}_i$ is given, after partial integration, by

$$\bar{I}_i(i\omega_n) = -(\tilde{\Gamma}/\pi) \int dE \frac{dN(E)}{dE} G(E, i\omega_n) \; . \tag{6.24}$$

Clearly no enhancement occurs for a constant $N(E)$. To provide an estimate of the magnitude of this correction we evaluate the lowest order correction $\delta\chi_i^{(1)}$, pictured in Fig. 8(d),

$$\begin{aligned}
\delta\chi_i^{(1)} &= 2\mu_B^2 (\tilde{\Gamma}/\pi) T \sum_n \sum_{kk'} G(k, i\omega_n)^2 G(k', i\omega_n)^2 \\
&= 2\mu_B^2 (\tilde{\Gamma}/\pi) \sum_{kk'} \frac{d}{dE_k} \frac{d}{dE_{k'}} T \sum_n G(k, i\omega_n) G(k', i\omega_n) \\
&\cong 2\mu_B^2 (\tilde{\Gamma}/\pi) \sum_{kk'} \frac{d}{dE_k} \frac{d}{dE_{k'}} \frac{1}{E_{k'} - E_k} T \sum_n [G(k, i\omega_n) - G(k', i\omega_n)] e^{i\omega_n \epsilon} \\
&= 2\mu_B^2 (\tilde{\Gamma}/\pi) \sum_{kk'} \frac{d}{dE_k} \frac{d}{dE_{k'}} \frac{f(E_k) - f(E_{k'})}{E_{k'} - E_k} \; .
\end{aligned} \tag{6.25}$$

The k dependence of the self-energy has been neglected in writing the energy denominator as $E_{k'} - E_k$. Using the isotropic approximation and performing partial integration in each variable gives

$$\delta\chi_i^{(1)} = 2\mu_B^2 \frac{\tilde{\Gamma}}{\pi} \int dE\, N'(E) \times \int dE' N'(E') \frac{f(E) - f(E')}{E' - E} \; . \tag{6.26}$$

We consider first the case where $N'(E) = dN(E)/dE$ can be taken to be constant in the important range around E_F. Setting

$$N'(E) = AN(E_F)/W \; , \tag{6.27}$$

where A is a constant of order unity and W is the bandwidth, leads to the result

$$\delta\chi_i^{(1)} = 2\mu_B^2 N(E_F) A^2 \frac{\ln 2}{\pi} \frac{\Gamma}{W} \; . \tag{6.28}$$

Thus defects may lead to a nonvanishing but usually small contribution to the Stoner I. For compounds with several transition-metal atoms per cell, however, W may represent a subband width such that Γ/W is not small, in which case it is necessary to do the integral in Eq. (6.26) more carefully. Nevertheless, we expect this contribution to χ generally to be secondary to the change in $N(E_F)$ in the simple bubble term due to defect broadening. Finally, it should be noted that this defect contribution to χ_{sp} need not always be positive as in Eq. (6.28). If E_F occurs at a peak, or a dip, in $N(E)$, in which case $N'(E)$ and $N'(E')$ in Eq. (6.26) have opposite signs in the important region of integration, the correction to χ_{sp} may be negative.

D. Interaction with phonons

It is not generally recognized that phonons can seriously alter the thermal occupation of crystalline eigenstates if the e-ph interaction is even moderately strong. It has been shown elsewhere[54] that e-ph interactions shift the spectral weight of low-energy electronic excitations drastically, and as a result the thermal occupation $f(E)$ broadens, corresponding to occupation of higher-energy bare electrons and holes. The resulting modification of the first term in Eq. (6.18) can be substantial. Since this effect of the e-ph interaction on $f(E)$, as well as many of its implications, is described elsewhere,[52] only phonon effects on the susceptibility will be addressed here.

Previous treatments[55,56] of the effect of e-ph interactions on the susceptibility have approached the problem from the viewpoint of a phonon contribution to the Stoner interaction parameter I. These treatments have all assumed a CDOS system, however, and in the general case it is not clear that this "Stoner I" viewpoint provides a useful approach. To see this, consider the Eq. (6.7′) neglecting the field dependence of the interaction: The frequency dependence of $\widetilde{\lambda}$ from the e-ph interaction is essential to the correct evaluation of this term and results in a *frequency-dependent enhancement* $J(i\omega_n)$. As a result J cannot be written in the simple (constant) form (6.20) as is the case for Coulomb interactions, nor even in the still simple (but frequency-dependent) form (6.23) as for defects.

We content ourselves here with studying briefly the first correction to χ_{sp} from e-ph interaction (beyond self-energy insertions to G). This correction is shown in Fig. 8(e) and is given by

$$\delta\chi^{(1)}_{e\text{-ph}}=2\mu_B^2T^2\sum_{\substack{kn\\k'n'}}G^2(k,i\omega_n)\widetilde{\lambda}(k-k';i\omega_n-i\omega_{n'})G^2(k',i\omega_{n'})\ . \tag{6.29}$$

In the isotropic approximation this becomes

$$\delta\chi^{(1)}_{e\text{-ph}}=2\mu_B^2T^2\sum_{nn'}\widetilde{\lambda}(i\omega_n-i\omega_{n'})\int dE\int dE'\,N'(E)G(E,i\omega_n)N'(E')G(E',i\omega_{n'})\ . \tag{6.30}$$

If $N(E)$ varies on the scale of Ω, no further simplification of this expression is possible. In particular, $\delta\chi^{(1)}_{e\text{-ph}}$ is not bounded in magnitude by any small parameter and it may be of either sign. Since this contribution to χ_{sp} is the first [Fig. 8(e)] in the e-ph ladder series leading to a generalized Stoner enhancement, the e-ph contribution to a "Stoner I" may be large and of either sign.

If $N'(E)$ can be approximated by a constant $N(E_F)/W$ over the range E_F-W to E_F+W, and is negligible otherwise, Eq. (6.30) can be evaluated for an Einstein phonon spectrum $\widetilde{\alpha}^2F(\omega)=(\widetilde{\lambda}\Omega_E/2)\delta(\omega-\Omega_E)$. The energy integral gives

$$\int dE\,N'(E)G(E,i\omega_n)\rightarrow -i\pi[N(E_F)/W]\,\text{sgn}\omega_n\ . \tag{6.31}$$

For $W \gg \Omega_E$ the frequency sums lead to the result

$$\delta\chi^{(1)}_{e\text{-ph}}\sim 2\mu_B^2N(E_F)\left[\frac{\lambda\Omega_E}{4W}\ln\frac{W}{\Omega_E}\right]\ , \tag{6.32}$$

suggesting that a ladder summation of such contributions would lead to a contribution to the Stoner I given by

$$I_{e\text{-ph}}\approx\frac{\lambda\Omega_E}{4W}\ln\frac{W}{\Omega_E}\ . \tag{6.33}$$

Oscillation in $N'(E)$ in transition-metal compounds is likely to severely reduce the dependence of $I_{e\text{-ph}}$ on the cutoff W, so the net result is likely to be dominated by DOS structure near E_F.

It is notable that Eq. (6.33) is of exactly the same form deduced by Fay and Appel[55] from the same diagram without invoking the isotropic approximation used here. Fay and Appel also emphasized that other diagrams may give phonon contributions to χ_{sp} of the same order as that resulting from Eq. (6.33). Although the contribution (6.30) to χ_{sp} is not bounded by any small quantity like Ω/W, there is still no assurance that other diagrams will not give important contributions. However, Eq. (6.30) has the advantage that the electron Green's function is dressed by phonons, implicitly accounting for an infinite subset of diagrams for χ_{sp}.

Kim,[56] taking another point of view, has considered the magnetic field dependence of the phonon frequencies arising from changes in electronic screening of the ion-ion interaction. The change $\Delta\omega_Q$ depends on the spin polarization, which may be Stoner-enhanced by the Coulomb interaction. Kim finds the result that the phonon contribution to I may itself be enhanced by the same factor, thereby greatly increasing the importance of $I_{e\text{-ph}}$ for nearly magnetic metals. Figure 8(c) gives the lowest-order diagram which arises from field dependence of the phonon spectrum. Recently MacDonald and Taylor[57] have suggested that refinements of Kim's theory will not lead to corrections as large as were envisioned by Kim.

E. Combined effects of interactions

A realistic calculation of χ_{sp} requires that all three of the interactions discussed above be taken into account simultaneously. The ladder diagrams, e.g., Fig. 7(b), can only be fully included by a numerical solution of Eq. (6.19), and corrections beyond the ladder approximation present additional difficulties. It might be expected that a reasonable first approximation would be to retain only the Coulomb part of $\tilde{\lambda}_{\text{eff}}$ in Eq. (6.19) but include defect and phonon contributions to G. The set of diagrams included in this approach is typified by the Coulomb ladder diagram of Fig. 8(f), and the corresponding contribution to χ_{sp} is given by

$$\chi_{\text{sp}}=2\mu_B^2 N_{\text{eff}}(\zeta)/[1-IN_{\text{eff}}(\zeta)] , \qquad (6.34)$$

with N_{eff} given by Eq. (6.21).

The results of the application of this expression, with I calculated from local-density-functional theory, have been described elsewhere.[58] It was found that, although the temperature dependence was qualitatively similar to the data of Reywald *et al.*,[59] both the calculated absolute magnitude and T dependence were only ~15% of the experimental values. The orbital susceptibility can certainly account for much of the discrepancy in magnitude, as well as for some of the T dependence which arises from the variation of ζ with temperature. However, it seems likely that disorder contributions to χ_{sp} other than those entering Eq. (6.30) through N_{eff} will be necessary for a more quantitative theory.

VII. CONCLUSION

A generalized formulation of the Eliashberg approach to the electron self-energy has been developed which is valid for crystals for which the electronic spectrum varies on the scale of phonon frequencies. The formulation has been kept on the imaginary frequency axis where it is numerically tractable, and further numerical application of the theory to $A15$ compounds will be presented elsewhere. Although there is no difficulty in extending the formalism to the real axis,[12,60] the resulting calculational difficulties make this approach unattractive when detailed results are wanted.

The present generalization of Eliashberg theory proposes a system of equations for describing the superconducting onset at T_c as well as the gap and renormalization functions below T_c. Calculations at and below T_c have shown that tunneling spectra[13,27] as well as thermodynamic behavior[60] can be significantly altered by DOS structure. In addition, it is proposed that the self-consistent approach of Eliashberg be extended above T_c to determine the *normal-state electronic self-energy.* This theory lays the foundation for a more unified picture of the relationship between high-temperature superconductivity and the anomalous normal-state behavior of $A15$ compounds, as in the conclusion that the temperature dependence of the susceptibility is increased substantially by the strong electron-phonon interaction.

The satisfying agreement between the calculational results discussed in Sec. V and the experimental data indicates that (1) the present proposal for the self-energy (Fig. 1) is adequate at low temperature, and (2) the DOS for Nb_3Sn calculated by Klein *et al.* is realistic. The disagreement between the theoretical and experimental susceptibility is certainly too large to be ascribed to an incorrect theoretical DOS function. A conceivable source of this discrepancy is that this *ansatz* for the self-energy is inadequate for temperatures approaching the Debye frequency; it is known (see Allen, Ref. 21) that even in CDOS systems there are further adiabatic corrections to Σ which cannot be shown to be small. However, I consider it more likely that the expression (6.34) for χ_{sp} is insufficient.

An important area which has not been addressed in this paper is the normal-state specific heat C_v, which has been used often to extract empirical values of $N(E_F)$. Let us assume, as the simplest situation, that the specific heat can be divided into electron and phonon contributions, as was shown to be the case for CDOS systems by Grimvall.[61] Generalizing Grimvall's general relation Eq. (A7) along the lines of the present theory leads to additional contributions to $C_{v,e}$ due to DOS variation, arising from the temperature variation of ζ and of $\gamma(\omega)$. Grimvall[61] has already concluded that $C_{v,e}$ is "far from linear at $T \simeq T_c$" for certain strong coupling superconductors. In addition, many A 15 compounds are known to have highly anharmonic phonons, which complicates the identification of $C_{v,\mathrm{ph}}$. Thus much theoretical work remains before the measured specific heat can be used to deduce detailed information about variation in $N(E)$.

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APPENDIX A

The usual expression[15,20] for the Coulomb pseudopotential $\bar{U}$ generalizes in the present case to

$$\bar{U}(k,k';0)=\bar{V}(k,k';0)+T\sum_{|\omega_n|>\omega_c}\sum_{k''}\frac{\bar{V}(k,k'';i\omega_n)\bar{U}(k'',k';0)}{[E_{k''}-\zeta+\chi(k'',i\omega_n)]^2+Z(k'',i\omega_n)^2[\omega_n^2+\Delta(k'',i\omega_n^2)]}\ . \tag{A1}$$

The treatment to this point ignores the possibility of spin fluctuation contributions and also assumes[15(c)] that $\bar{V}$ is essentially positive, eliminating the consideration of enhancement of superconductivity by plasmon or exciton mechanisms. In principle, the dynamically screened Coulomb interaction $\bar{V}$ includes Coulomb renormalization and Coulomb vertex corrections.

For the "frequencies" ω_n and energies $E_{k''}$ of interest in Eq. (A1) it suffices to ignore the self-energy corrections to the denominator. Performing the energy surface averages leads to

$$\tilde{\mu}^*(E,E')=\tilde{\mu}(E,E')+T\sum_{|\omega_n|>\omega_c}\int dE''\tilde{\mu}(E,E'')\frac{N(E'')}{E''^2+\omega_n^2}\tilde{\mu}^*(E'',E')\ . \tag{A2}$$

To make contact with later notation $\tilde{\mu}^*(E,E') \equiv \bar{U}(E,E';0)$ and $\tilde{\mu}(E,E') \equiv \bar{V}(E,E';0)$ have been introduced, and also the frequency dependence of $\bar{V}$ has been ignored.

Assuming further that

$$\tilde{\mu}(E,E')=\begin{cases}\tilde{\mu}, & |E|,|E'|<\omega_{\mathrm{pl}}\\ 0 & \text{otherwise}\end{cases} \tag{A3}$$

and that $N(E)$ vanishes for $|E|>\omega_{\mathrm{pl}}$, one finds

$$1/\tilde{\mu}^*=1/\tilde{\mu}+L(\omega_c,\omega_{\mathrm{pl}})\ , \tag{A4}$$

where

$$L(\omega_c,\omega_{\mathrm{pl}})\equiv T\sum_{|\omega_n|>\omega_c}\int_{-\omega_{\mathrm{pl}}}^{\omega_{\mathrm{pl}}}dE\frac{N(E)}{E^2+\omega_n^2}\ . \tag{A5}$$

For a specific model of $N(E)$, L can be evaluated explicitly. Given the level of approximation leading to Eq. (A4) however, it suffices to note that

$$L(\omega_c,\omega_{\mathrm{pl}})\approx\bar{N}(\omega_{\mathrm{pl}})l(\omega_c,\omega_{\mathrm{pl}})$$
$$\approx\bar{N}(\omega_{\mathrm{pl}})\ln(\omega_{\mathrm{pl}}/\omega_c)\ , \tag{A6}$$

where $\bar{N}(\omega_{\mathrm{pl}})$ is the mean DOS over a region $E_F \pm \omega_{\mathrm{pl}}$ and $l(\omega,\omega')$ (introduced by Allen[15(e)]) is the function $L(\omega,\omega')$ with $N(E)$ replaced by unity. In the (strict) CDOS limit $\bar{N}(\omega_{\mathrm{pl}}) \rightarrow N(E_F)$, the usual expression

$$1/\mu^*=1/\mu+\ln(\omega_{\mathrm{pl}}/\omega_c) \tag{A7}$$

is recovered, where $\mu=N(E_F)\tilde{\mu}$ and $\mu^*=N(E_F)\tilde{\mu}^*$. However, the CDOS limit of Eliashberg theory applies if $N(E)$ is approximately constant over the range $E_F \pm \omega_c$, in which case a more precise expression for μ^* is given by

$$1/\mu^*=1/\mu+[\bar{N}(\omega_{\mathrm{pl}})/N(E_F)]\ln(\omega_{\mathrm{pl}}/\omega_c)\ . \tag{A8}$$

This relation is discussed further in the text.

APPENDIX B

The calculations described in this paper require the self-consistent solution of the $N_c \times N_c$ matrix equations (2.5), (3.12), and (4.1)−(4.3). Two techniques used in the present computations will be described briefly here.

These equations have the feature that the low-frequency (small $|\omega_n|$) rows and columns are in some sense more critical for obtaining convergence than those of larger frequency. It has been found that the technique used by Allen[62] of using the solution of the $m \times m$ subsystem as an approximate solution of a larger subsystem provides an efficient method of providing an iterative solution of the system of equations. The sequence $m = 1,2,4,8,\ldots,N_c$ used by Allen has been used here, with $N_c = 128$ for all calculations described in this paper.

The only arbitrary assignments in this procedure occur in setting initial values of N_n and P_n. The iteration is begun by setting $N_0 = N(E_F)$, $P_0 = 0$, then calculating Z_0, χ_0, Δ_0, and $\zeta^{(0)}(T)$, the first approximation to $\zeta(T)$ (see below). Then N_0 and P_0 are recalculated until self-consistency is obtained. In proceding from the solutions of $m \times m$ subsystem to the $2m \times 2m$ subsystem, the assignment

$$\begin{Bmatrix} N_j \\ P_j \end{Bmatrix} = \begin{Bmatrix} N_m \\ P_m \end{Bmatrix}, \quad m < j \leq 2m \tag{B1}$$

was made. A search for more sophisticated extrapolations of these functions did not result in significantly more efficient solutions.

A crucial step in attaining reasonably accurate solutions to this system is finding a procedure for determining $\zeta(T)$ from Eq. (2.5). The free Green's function G_0, for instance, gives rise to the Fermi-Dirac distribution function f_0

$$f_0(E) = T \sum_n G_0(E, i\omega_n) e^{i\omega_n \epsilon} \tag{B2}$$

only after an *infinite summation;* truncation of the frequency sum in Eq. (B2) at any point leads to a function which is nonexponential. In the present calculation ζ has been evaluated as follows.

For the $m \times m$ subsystem, $m = 1,2,4,\ldots,N_c$, we make the definition

$$Z_j = \Delta_j = \chi_j = 0, \quad j > m \ . \tag{B3}$$

Then Eq. (2.5) can be written

$$\begin{aligned} N_e &= 2T \sum_{n \geq 0} \int dE\, N(E) \mathrm{Re} G(E, i\omega_n; \zeta) e^{i\omega_n \epsilon} \\ &= 2T \,\mathrm{Re} \int dE\, N(E) \sum_{n \geq 0} \{ G_0(E, i\omega_n; \zeta) + [G(E, i\omega; \zeta) - G_0(E, i\omega; \zeta)] \} \\ &= 2 \int dE\, f_0(E - \zeta) N(E) + 2T \,\mathrm{Re} \sum_{n=0}^{m} \int dE\, N(E) [G(E, i\omega_n; \zeta) - G_0(E, i\omega_n; \zeta)] \ . \end{aligned} \tag{B4}$$

The relation $G(E, -i\omega_n) = G(E, i\omega_n)^*$ has been used in writing the sums over $\omega_n > 0$ only. The dependence on ζ, the *interacting chemical potential,* has been displayed explicitly to emphasize that introducing $G_0(E, i\omega_n; \zeta)$ and $f_0(E - \zeta)$ is merely a mathematical method for evaluating the infinite summation. In particular,

$$2 \int dE\, f_0(E - \zeta) N(E) \neq N_e \ . \tag{B5}$$

Finally, *the noninteracting chemical potential* $\zeta_0(T)$, determined by

$$N_e = \int dE\, f_0(E - \zeta_0) N(E) \ , \tag{B6}$$

was used to write the equation determining ζ as

$$2T \,\mathrm{Re} \sum_{n=0}^{m} \int dE\, N(E) [G(E, i\omega_n; \zeta) - G_0(E, i\omega_n; \zeta)] = 2 \int dE\, [f_0(E - \zeta_0) - f_0(E - \zeta)] N(E) \ . \tag{B7}$$

This equation is solved iteratively for ζ at each step of the iteration of the system of equations.

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