Effect of d-wave energy-gap symmetry on Raman shifts

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We have calculated the shift and change in width, due to superconductivity, for a $\mathbf{q}=\mathbf{0}$ Raman-active phonon in a two-dimensional, tight-binding band structure with a d-wave pairing interaction. We find that additional structure appears in the phonon self-energy due to the van Hove singularity, which occurs in two dimensions. A more general model of a superconductor with nodes in the gap function is also examined and related to both the d-wave model and another model for layered superconductors. In contrast to the usual isotropic s-wave case where a phonon with frequency less than twice the gap value is softened and narrowed, we find softening with broadening in these models. Comparison of the anisotropic models is made with experiment.

I. INTRODUCTION

While the mechanism for superconductivity in the high-T_c oxides remains an open question, there is growing interest in the possibility of the pairing interaction exhibiting non-s-wave symmetry. Such an explanation is persuasive, as other exotic superconductors, such as the heavy-fermion and organic superconductors, are now thought to be possibly described in terms of d-wave or unconventional pairing. For the high-T_c oxides, the experimental evidence for quasiparticle states extending down to zero frequency inside a supposed gap region supports the idea of nodes existing in the gap function. Experimental evidence for states within the gap include tunneling,[1] optical conductivity,[2] Raman intensity,[3] and penetration depth,[4] to name a few. Other support for a pairing interaction with nodes comes from the unusual NMR relaxation rate as a function of temperature below T_c. In particular, the ratio of the relaxation rate in the a-b plane to that in the c direction in $YBa_2Cu_3O_7$ displays an unusual S shape which has only found explanation, at present, in terms of a d-wave model with the existence of nodes.[5–7] Hence it is of interest to study the effect of different gap symmetries on various superconducting properties to look for signatures which may be defined in experiment.

In this paper we wish to examine how nodes in the gap function affect Raman phonon shifts and widths. To this end we will focus on the d-wave symmetry of the gap function, although we will show our results are more generally applicable to nodes in the gap function. The motivation for choosing the d-wave symmetry arises from theoretical results based on two-dimensional Hubbard-model calculations which appear to favor this symmetry.[8] In addition, Pines and co-workers[9,10] have proposed a phenomenological model for antiferromagnetic paramagnons in the Cu-O planes giving rise to $d_{x^2-y^2}$ symmetry.[10] Their model is based upon examination of the NMR relaxation-rate experiments and deducing from them a susceptibility which pairs in the d-wave channel. Here we will not espouse a specific interaction, but rather will choose to use the gap symmetry corresponding to this $d_{x^2-y^2}$ state and work within a BCS model. We will comment briefly on results of strong-coupling calculations at the end of the paper.

II. THEORY

Following the lead of many authors on this subject and, in particular, the notation of Zhou and Schulz,[11] we base our work on a two-dimensional tight-binding model on a square lattice with nearest-neighbor interactions. The mean-field Hamiltonian in this model for superconductivity with spin-singlet pairing is given as

$$H=\sum_{\mathbf{k}\sigma}\varepsilon_{\mathbf{k}}a^{\dagger}_{\mathbf{k}\sigma}a_{\mathbf{k}\sigma}+\sum_{\mathbf{k}}(\Delta_{\mathbf{k}}a^{\dagger}_{\mathbf{k}\uparrow}a^{\dagger}_{-\mathbf{k}\downarrow}+\text{H.c.}) , \tag{1}$$

where the dispersion relation for nearest-neighbor interactions on a square lattice is given by

$$\varepsilon_{\mathbf{k}}=-2t[\cos(k_x a)+\cos(k_y a)]-\mu . \tag{2}$$

Here a is the lattice spacing, $a^{\dagger}_{\mathbf{k}\sigma}$ ($a_{\mathbf{k}\sigma}$) is the creation (annihilation) operator for a particle with spin σ and momentum $\mathbf{k}$, μ is the chemical potential, and t is the hopping parameter. The above energy dispersion corresponds to a bandwidth of $8t$. The anisotropic gap parameter $\Delta_{\mathbf{k}}$ is solved self-consistently from

$$\Delta_{\mathbf{k}}=\frac{1}{N}\sum_{\mathbf{k}'}V_{\mathbf{k}\mathbf{k}'}\langle a_{-\mathbf{k}'\downarrow}a_{\mathbf{k}'\uparrow}\rangle$$
$$=\frac{T}{N}\sum_{n}\sum_{\mathbf{k}'}V_{\mathbf{k}\mathbf{k}'}\frac{\Delta_{\mathbf{k}'}}{\varepsilon^2_{\mathbf{k}'}+\omega_n^2+\Delta^2_{\mathbf{k}'}} , \tag{3}$$

where N is the number of sites, T is the temperature, and ω_n is the fermion Matsubara frequency. In this expression the pairing interaction must be specified, which, in a BCS approximation, we choose to be

$$V_{\mathbf{k}\mathbf{k}'}=-V\eta_{\mathbf{k}}\eta_{\mathbf{k}'} , \tag{4}$$

where, for the symmetry of interest here,

$$\eta_{\mathbf{k}}=\cos(k_x a)-\cos(k_y a) . \tag{5}$$

This leads to a solution for $\Delta_{\mathbf{k}}$ of the form

$$\Delta_{\mathbf{k}}=\Delta\eta_{\mathbf{k}}=\Delta[\cos(k_x a)-\cos(k_y a)] , \tag{6}$$

which gives a maximum gap of 2Δ. Lines of nodes occur in the gap function along the direction $(\pm,\pi/a,\pm\pi/a)$ in the Brillouin zone.

Gap anisotropy effects with relation to the Raman cross section have been previously discussed by Abrikosov and Falkovsky[12] and Monien and Zawadowski.[13] The purpose of this paper is to answer the following question: In comparison with s-wave superconductivity, how does a d-wave symmetry (or, more generally, a superconductor with nodes in the gap function) affect the shifts and widths of phonons observed in Raman light-scattering experiments. The phonon self-energy at $\mathbf{q}=0$ has been calculated for the high-T_c oxides assuming s-wave pairing by Zeyher and Zwicknagl[14] and Marsiglio, Akis, and Carbotte.[15] An electronic mechanism has been investigated by Nicol and Carbotte.[16] Arguments for the justification of these calculations have been set forth in the papers of Zeyher and Zwicknagl.[14] The Zeyher-Zwicknagl theory[14] has been used by many experimentalists in an attempt to extract an energy gap from the data.[17] The question one might ask is, how would the experimental interpretation of the data change if the symmetry of the pairing interaction is d wave? Could a feature still be identified as being related to the energy gap? We will attempt to answer these questions here.

Following the work of Zeyher and Zwicknagl,[14] the phonon self-energy, assuming a polarization bubble with no vertex corrections, is given by

$$\Sigma_\lambda(\mathbf{q};i\nu_n)=\frac{T}{N}\sum_{\mathbf{k}}\sum_{m}|g_\lambda(\mathbf{k},\mathbf{k}+\mathbf{q})|^2\mathrm{Tr}\{\tau_3 G[\mathbf{k}+\mathbf{q},i(\omega_n+\nu_n)]\tau_3 G(\mathbf{k},i\omega_m)\} , \tag{7}$$

where τ_3 is a Pauli matrix, $G(\mathbf{k},i\omega_m)$ is the fully interacting Green's function, ω_m (ν_n) is the fermion (boson) Matsubara frequency, and $g_\lambda(\mathbf{k},\mathbf{k}+\mathbf{q})$ is the electron-phonon matrix element for scattering of an electron of momentum $\mathbf{k}$ to $\mathbf{k}+\mathbf{q}$ with momentum transfer $\mathbf{q}$ to or from a phonon with branch index λ. In BCS theory the superconducting Green's function is

$$G(\mathbf{k},i\omega_n)=-\frac{i\omega_m+\varepsilon_{\mathbf{k}}\tau_3+\Delta_{\mathbf{k}}\tau_1}{\varepsilon_{\mathbf{k}}^2+\omega_m^2+\Delta_{\mathbf{k}}^2} . \tag{8}$$

Substitution of Eq. (8) into Eq. (7) and taking $\mathbf{q}=0$ yields

$$\Sigma_\lambda(i\nu_n)=-\frac{4}{N}\sum_{\mathbf{k}}\tanh\left[\frac{E_{\mathbf{k}}}{2T}\right]\frac{\Delta_{\mathbf{k}}^2|g_{\lambda\mathbf{k}}|^2}{E_{\mathbf{k}}[(2E_{\mathbf{k}})^2+\nu_n^2]} , \tag{9}$$

where $E_{\mathbf{k}}=(\varepsilon_{\mathbf{k}}^2+\Delta_{\mathbf{k}}^2)^{1/2}$ and $g_{\lambda\mathbf{k}}\equiv g_\lambda(\mathbf{k},\mathbf{k})$. The usual quantity to show is the difference between the superconducting and normal-state self-energies,

$$\Delta\Sigma(i\nu_n)=\Sigma^S(i\nu_n)-\Sigma^N(i\nu_n) ,$$

where Σ^N is obtained from Eq. (9) by setting $\Delta=0$. In the case of the above expression, which is for the clean limit (i.e., no impurity scattering), $\Sigma^N=0$. $\Delta\Sigma(i\nu_n)$ is then analytically continued ($i\nu_n\rightarrow\nu+i\delta$), and the real part describes the shifts in phonon frequencies and the imaginary part describes the change in phonon widths upon entering the superconducting state.

The simplest method for evaluating Eq. (9) for the band structure given in Eq. (2) and the gap parameter given in Eq. (6) is to numerically evaluate Eq. (9) on a lattice.[18] We have done so in this paper.

The band structure of Eq. (2) in two dimensions gives rise to a van Hove singularity in the electronic density of states,

$$N(\omega)=\frac{1}{N}\sum_{\mathbf{k}}\delta(\omega-E_{\mathbf{k}}) . \tag{10}$$

If one is willing to sacrifice an exact evaluation of Eqs. (9), (2), and (6), an approximation can be made that will reduce the number of integration variables by 1 facilitating the more numerically intensive Eliashberg strong-coupling calculation. A transformation is employed of the form[10]

$$\cos(k_x a)=-\varepsilon-(1-|\varepsilon|)\cos\theta , \tag{11}$$

$$\cos(k_y a)=-\varepsilon+(1-|\varepsilon|)\cos\theta , \tag{12}$$

for $-1\le\varepsilon\le 1$ and $0\le\theta\le\pi$. This transformation maps out constant-energy ε surfaces in the first quadrant of the square Brillouin zone. Assuming that t is very large and can be taken to infinity and that we are at a filling where we are far away from the van Hove singularity such that we can assume a constant density of states around the Fermi level, which will be

$$N(0)\approx\frac{1}{2\sqrt{2}\pi t|\bar{\mu}|^{1/2}} , \tag{13}$$

$[\bar{\mu}\equiv\mu/(2t)]$, then

$$\Delta\Sigma_\lambda(i\nu_n)=-\frac{4N(0)}{\pi}\int_0^\pi d\theta\int_{-\infty}^{+\infty}d\varepsilon\tanh\left[\frac{E}{2T}\right]\times\frac{\Delta_\theta^2|g_{\lambda\theta}|^2}{E[(2(E)^2+\nu_n^2]} . \tag{14}$$

Here $E=(\varepsilon^2+\Delta_\theta^2)^{1/2}$, $g_{\lambda\theta}$ is the electron-phonon matrix element in these new variables with the assumption that this quantity will only depend upon the angle but not on the energy, and

$$\Delta_\theta=\Delta\alpha\cos\theta , \tag{15}$$

with

$$\alpha=-(2-|\bar{\mu}|) . \tag{16}$$

Under this approximation the problem has been reduced

to a gap parameter of the form $\Delta_\theta=\Delta\alpha\cos\theta$ with only one integration variable, as the ε integral can be done analytically in most cases. This is much easier to handle numerically for Eliashberg strong-coupling calculations and is also a more general form of a gap parameter which exhibits nodes. This expression is particularly simple for the real part at $T=0$ and for the imaginary part at any temperature, as it can be reduced analytically to[15]

$$\frac{\Delta\Sigma_\lambda(\nu+i\delta)}{N(0)}=\frac{1}{\pi}\int_0^\pi d\theta|g_{\lambda\theta}|^2\frac{\Delta\Sigma_\theta(\nu+i\delta)}{N(0)}\ , \tag{17}$$

where

$$\frac{\mathrm{Re}\Delta\Sigma_\theta(\nu+i\delta)}{N(0)}=\begin{cases}-\dfrac{2}{\bar\nu(1-\bar\nu^2)^{1/2}}\tan^{-1}\left[\dfrac{\bar\nu}{(1-\bar\nu^2)^{1/2}}\right] & \text{for } \bar\nu<1\ ,\\ \dfrac{1}{\bar\nu(\bar\nu^2-1)^{1/2}}\ln[2\bar\nu^2-1+2\nu(\bar\nu^2-1)^{1/2}] & \text{for } \bar\nu>1\ ,\end{cases} \tag{18}$$

$$\frac{\mathrm{Im}\Delta\Sigma_\theta(\nu+i\delta)}{N(0)}=\begin{cases}0 & \text{for } \bar\nu<1\ ,\\ -\pi\dfrac{\tanh(\nu/4T)}{\bar\nu(\bar\nu^2-1)^{1/2}} & \text{for } \bar\nu>1\ ,\end{cases} \tag{19}$$

where $\bar\nu_\theta\equiv\nu/(2\Delta_\theta)$. This form can be easily implemented for model fits to data. Using any general choice of symmetry for the gap function, Eqs. (17)–(19) can be evaluated using the appropriate angular integration (within a constant density-of-states approximation). While the form of Eqs. (15) and (16) contains the physics of Eq. (6), with $\alpha=1$, it is also equivalent (in the limit of large anisotropy in the gap parameter) to the form obtained for an anisotropic layered superconductor with anisotropy in the z direction.

In this model of a layered superconductor, which has been studied extensively in the context of copper oxide superconductivity by many authors,[19–26] electrons hop between planes with a hopping parameter t and propagate freely in the planes. The dispersion relation for the electrons is given as

$$\varepsilon_{\mathbf{k}}=\frac{1}{2m^*}(k_x^2+k_y^2)+\frac{t}{m^*}\cos(k_zc)\ , \tag{20}$$

with c the lattice constant in the direction perpendicular to the planes and m^* the effective mass. This band structure yields an open, hour-glass-shape Fermi surface for the Fermi energy $\varepsilon_F>t/m^*$.[26] In this limit the density of states is constant and a gap ansatz is used, which is of the form

$$\Delta_{\mathbf{k}}=\Delta[1+b\cos(k_zc)]\ . \tag{21}$$

Here b is the anisotropy parameter, with $b=0$ corresponding to pure s-wave symmetry. In this model we can once again evaluate Eq. (14) with

$$\Delta_\theta=\Delta(1+b\cos\theta)\ . \tag{22}$$

When b is very large, this model approaches the $\alpha\Delta\cos\theta$ form.

In the following we will present the phonon self-energy for the $d_{x^2-y^2}$ model. We will then compare this model with the $\alpha\Delta\cos\theta$ model to demonstrate what features have been lost in the approximations. The $\alpha\Delta\cos\theta$ form will then be used to compare with the standard s-wave calculation and to make general statements about gap structure with nodes. Finally, we will exhibit results for the gap symmetry relevant for a layered superconductor and demonstrate that, with large anisotropy, it approximates a gap function with nodes.

III. RESULTS

A. d-wave symmetry: $\Delta_{\mathbf{k}}=\Delta[\cos(k_xa)-\cos(k_ya)]$

The first result that we will exhibit is the exact evaluation of the phonon self-energy given in Eq. (9) at zero temperature using the gap ansatz of Eq. (6) and the band structure of Eq. (2). We have also taken $g_{\mathbf{k}}\propto\eta_{\mathbf{k}}$, assuming that the electron-phonon interaction exhibits the same anisotropy as the interaction which renormalizes the electron Green's function in the superconducting state. (We will have more to say about this further on). The calculation was done on a lattice,[18] and therefore the curves exhibit some rounding due to finite-size effects. The results are shown in Fig. 1. The upper frame is the real part of the phonon self-energy, corresponding to shifts in the phonon frequency, and the lower frame is the imaginary part, commenting on changes of phonon widths or, equivalently, lifetime effects. Curves are shown for different $\bar\mu$ (which can be related to the filling factor) as labeled in the figure caption. In this figure, $\bar\Delta\equiv\Delta/(2t)=0.1$, $t=1.0$ eV, and we have used a lattice size of 1024×1024 with $\delta=0.008$ ($i\nu_n\rightarrow\nu+i\delta$). Throughout this paper Δ_0 refers to the zero-temperature value of Δ. At half-filling (i.e., $\bar\mu=0$), a phonon with frequency below $4\Delta_0$ (or twice the maximum gap) softens, while above $4\Delta_0$ it would be hardened, with considerable hardening just above $4\Delta_0$. As we move away from half-filling, hardening can occur for frequencies as low as $\nu\sim2\Delta_0(2-|\bar\mu|)$ and the sharp peak structure at $4\Delta_0$ diminishes and moves to higher frequency. To understand fully this structure, it is better to look at the imaginary part of the self-energy for the change in phonon widths and compare this to the density of states. The real part is

related to the imaginary part of the phonon self-energy by Kramers-Kronig transformation.

In the imaginary part of the phonon self-energy (bottom frame of Fig. 1), the phonon is always broadened in the superconducting state with greater broadening occurring in two places. These two positions of increased broadening can be understood from an examination of the corresponding density of states shown in Fig. 2. The density of states shown here was evaluated from Eq. (10) by a lattice calculation and for the same parameters as shown in Fig. 1. Zhou and Schulz[11] have already performed a similar calculation for this quantity and have given a very thorough discussion of the features observed here. We summarize here their main results. There is a finite number of quasiparticle states at all frequencies, with a linear variation in frequency as $\omega \to 0$. The first peak at low frequency is due to the superconductivity and is a logarithmic divergence rather than the usual square-root divergence. This is due to the two dimensionality. This frequency corresponds to $\omega_1 = 2t\bar{\Delta}(2+\bar{\mu})/(1+\bar{\Delta}^2)^{1/2}$ [$\simeq 2t\bar{\Delta}(2+\bar{\mu})$ for $\bar{\Delta} \equiv \Delta/(2t) \ll 1$]. The higher-energy peak is due to the van Hove singularity

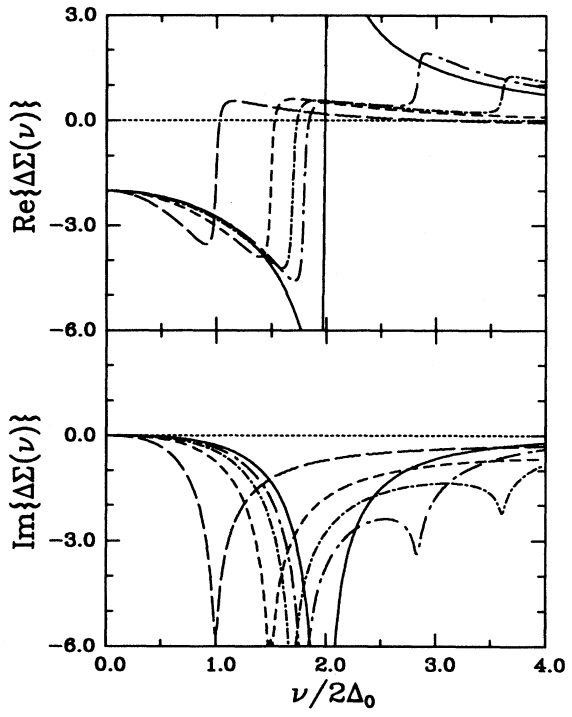

FIG. 1. $\mathbf{q}=0$ phonon self-energy, in BCS theory, at zero temperature and in the clean limit for the d-wave model described in the text. The top frame is the real part, and the bottom frame is the imaginary part. The curves have been normalized to give the usual zero-frequency limit for the real part. This calculation has been performed on a lattice with the parameters given in the text. Curves are drawn for $\bar{\mu}=0.0$ (solid curve), -0.2 (dot-long-dashed curve), -0.3 (dot-short-dashed curve), -0.5 (short-dashed-curve), and -1.0 (long-dashed-curve). Negative (positive) values correspond to softening (hardening) in the top frame and broadening (sharpening) in the bottom frame.

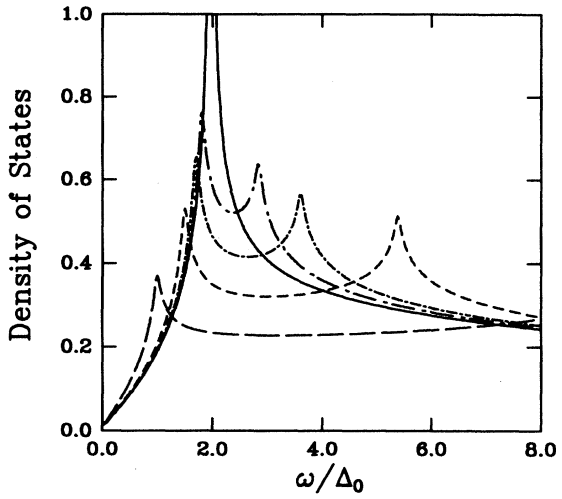

FIG. 2. Quasiparticle density of states calculated on a lattice for the d-wave model discussed in the text. Curves are drawn for $\bar{\mu}=0.0$ (solid curve), -0.2 (dot-long-dashed curve), -0.3 (dot-short-dashed curve), -0.5 (short-dashed-curve), and -1.0 (long-dashed curve). The same parameters are used as for Fig. 1. The lower-frequency peak corresponds to the superconducting singularity, and the higher-frequency peak corresponds to the van Hove singularity which occurs in two dimensions. At $\bar{\mu}=0$ the two peaks combine into one.

which always occurs in two dimensions. For $|\bar{\mu}|/2 < \bar{\Delta}^2$ it is positioned at $\omega_2 = 2t\bar{\Delta}(2-\bar{\mu})/(1+\bar{\Delta}^2)^{1/2}$ and for $|\bar{\mu}|/2 > \bar{\Delta}^2$ (the expected situation in the high-T_c oxides) $\omega_2 = 2t(\bar{\mu}^2+4\bar{\Delta}^2)^{1/2}$. If $\bar{\mu}=0$, both peaks combine into one peak at $\omega = 2\Delta$. (Note that in Fig. 2 the peaks are not as sharp as they should be because of the fact that the calculation was done on a finite-size lattice.) We see very clearly a reflection of this density of states in the imaginary part of $\Delta\Sigma$ with the dips occurring at twice the frequencies of the peaks in Fig. 2. This is a result of the process whereby the phonon scatters with a particle-hole pair and is broadened. This particle-hole pair may be created only at $\omega \geq 2\Delta_0$ in an s-wave superconductor as two quasiparticles must be liberated from the superconducting condensate, costing a minimum in energy of $2\Delta_0$. However, in a superconductor with nodes in the gap function, particle-hole pairs can be created at arbitrarily low energy (at the nodes) and contribute to scattering. Likewise, at the peaks in the quasiparticle density of states, more quasiparticle scattering is available to relax the phonon with a factor of 2 showing up in the self-energy as, in all instances, both a particle and a hole must be created. The main conclusion of the overall discussion here is that for a d-wave superconductor there is a region in which a phonon will be broadened and softened which is unlike the behavior of an s-wave superconductor, as we will shortly discuss.

B. General gap anisotropy with nodes: $\Delta_\theta = \alpha\Delta\cos\theta$

In Fig. 3 we display the result of evaluating the phonon self-energy in the constant density-of-states approxima-

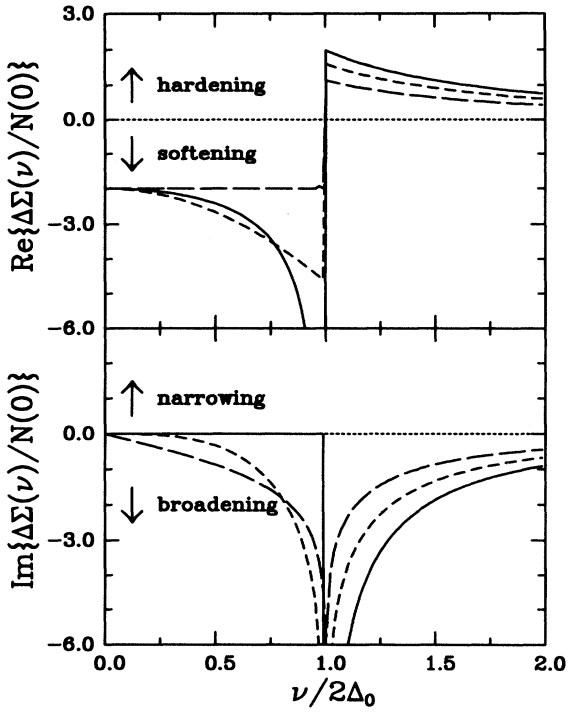

FIG. 3. q=0 phonon self-energy, in BCS theory, at zero temperature and in the clean limit for three cases. The solid curve is the s-wave result (Refs. 14–16). The short-dashed curve corresponds to the $\alpha\Delta\cos\theta$ model with $\alpha=1$ and g_k taken to be proportional to $\alpha\cos\theta$. And the long-dashed curve illustrates the same model as the short-dashed curve, but with g_k taken to be a constant. The top frame is the real part, and the bottom frame is the imaginary part. This calculation has not been performed on a lattice, but evaluated numerically by a standard integration routine. Here it is clearly illustrated that only for the gap function with nodes can there be the possibility of softening accompanied by broadening.

tion of Eq. (14) with $T=0$, which reduces to the very simple result of Eq. (17). For this calculation and all that follows hereafter, we have not done a lattice calculation as the integrals are easily solved by exact numerical integration. Here we take $\alpha=1$, which corresponds to $\bar{\mu}=-1$. The solid curve is the BCS s-wave result in three dimensions, the short-dashed curve is the $\alpha\Delta\cos\theta$ model with $g_\theta\propto a\cos\theta$, and the long-dashed curve is for the $\alpha\Delta\cos\theta$ model with g_θ equal to a constant (i.e., in this latter instance, we assume that the anisotropy in the superconducting pairing interaction is completely unrelated to the electron-phonon coupling). First, comparing the result of the short-dashed curve (the $\alpha\Delta\cos\theta$ model) with the corresponding $\bar{\mu}=-1$ curve of Fig. 1 (the long-dashed curve), we see that other than a small overall magnitude factor (related to the choice of $\bar{\Delta}$ in Fig. 1), the curves are essentially the same, indicating that the constant density-of-states approximation is good for $\bar{\mu}$ away from zero (away from half-filling). The main feature not captured by the approximation as $\bar{\mu}$ approaches zero is the higher-frequency structure due to the van Hove singularity. This is not surprising as the approximation neglects the van Hove singularity entirely. It is also not a great loss as the singularity is somewhat artificial since three-dimensional effects, strong-coupling effects, etc., are likely to smear and reduce it considerably.[27] The $\alpha\Delta\cos\theta$ form, however, correctly captures the singularity due to the superconductivity which occurs at $\nu=2\Delta_0(2-|\bar{\mu}|)$. In the constant density-of-states approximation, changing $\bar{\mu}$ merely scales the x axis on the curves in Fig. 3 to maintain the singularity at $\nu=2\Delta_0(2-|\bar{\mu}|)$. Note that the singularity always occurs at twice the *maximum gap* [i.e., $2\Delta_0$ for Eq. (6)] *minus* $2\Delta_0|\bar{\mu}|$ which corresponds to the maximum gap on the Fermi surface. If the electron-phonon coupling has no anisotropy, as might be the case if the superconductivity is due to a mechanism other than electron-phonon coupling, the effect is primarily to reduce the amount of softening near $2\Delta_0$ (long-dashed curve). The main feature of this figure is the comparison between the case of nodes in the gap function and s-wave superconductivity (that is, no nodes). According to Fig. 3, in s-wave superconductivity a phonon with frequency below $2\Delta_0$ will soften and not be altered in width (or be narrowed in the case of impurity scattering). For a superconductor with nodes in the gap function (d-wave or otherwise), a phonon can be broadened and softened in the superconducting state.

In Fig. 4, we show the same case as for the short-

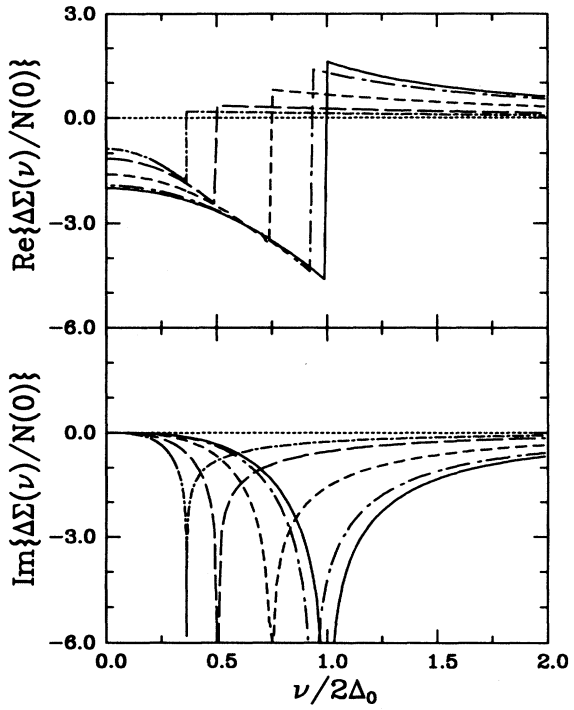

FIG. 4. q=0 phonon self-energy, in BCS theory, at finite temperature and in the clean limit for the case of the $\alpha\Delta\cos\theta$ model with anisotropy in the electron-phonon coupling $g_k\propto\alpha\cos\theta$. Curves are drawn for $T/T_c=0.0$ (solid curve), 0.5 (dot-long-dashed curve), 0.75 (short-dashed curve), 0.9 (long-dashed curve), and 0.95 (dot-short-dashed curve). Again, negative (positive) values corresponding to softening (hardening) in the top frame and broadening (sharpening) in the bottom frame.

dashed curve of Fig. 3 (the $\alpha\Delta\cos\theta$ form with anisotropy in g_θ) but now for several temperatures below T_c, with the temperature dependence of the gap parameter solved self-consistently from Eq. 3 with $\varepsilon_k=\varepsilon$ and $\Delta_k=\alpha\Delta\cos\theta$,

$$\frac{1}{N}\sum_k \rightarrow \frac{N(0)}{\pi}\int_{-\infty}^{\infty} d\varepsilon \int_0^{\pi} d\theta \ .$$

The anisotropy slightly reduces the temperature dependence of the gap function below that of BCS.[28] With increasing temperature the curves decrease in magnitude and shift to the left as the gap closes, with the singularity always tracking $\Delta(T)$. Softening with broadening always remains as a feature for phonons with energy below $2\Delta(T)$.

C. Layered superconductors: $\Delta_{k_z}=\Delta[1+b\cos(k_z c)]$

In Fig. 5 we display the results for the phonon self-energy in the model of a layered superconductor at $T=0$, with an anisotropic gap function $\Delta_k=\Delta[1+b\cos(k_z c)]$. We have also used the same anisotropy in the electron-phonon interaction $g_{k_z}\propto 1+b\cos(k_z c)$. Curves are drawn for different values of the anisotropy parameter b as indicated in the figure caption. For $b=0$ the standard isotropic s-wave result is recovered (solid curve). For $b\neq 0$ there exist three regions of behavior. For frequencies below twice the minimum gap, the behavior is entirely s-wave-like, with softening accompanied by no change in phonon width. In the region corresponding to $2\Delta(1-b)<\nu<2\Delta(1+b)$, i.e., bounded by twice the minimum and maximum gaps, the behavior is like that for a gap parameter with nodes (i.e., the $\alpha\Delta\cos\theta$ model). Here, once again, we see a region of softening with broadening. Finally, for frequencies above twice the maximum gap, the behavior is similar to both s- and d-wave behavior for high frequencies, i.e., broadening with hardening. In this model, therefore, it is also possible to have a region of frequency where a phonon could be softened and broadened, due to the d-wave-like piece in the gap function.

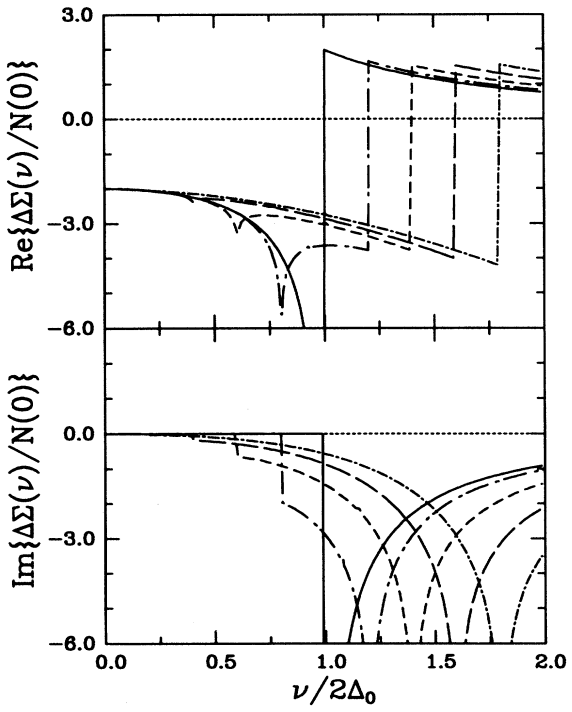

FIG. 5. $\mathbf{q}=0$ phonon self-energy, in BCS theory, at zero temperature and in the clean limit for a model pertinent to layered superconductors with gap anisotropy given by $\Delta_k=\Delta_0[1+b\cos(k_z c)]$. Here we have taken g_k to be proportional to $1+b\cos(k_z c)$. The top frame is the real part, and the bottom frame is the imaginary part. Curves are drawn for different values of the anisotropy parameter b: $b=0$ or s wave (solid curve), 0.2 (dot-long-dashed curve), 0.4 (short-dashed curve), 0.6 (long-dashed curve), and 0.8 (dot-short-dashed curve). For large anisotropy the curves approach those of the $\alpha\cos\theta$ model in Fig. 3.

Note that as the anisotropy parameter b increases, the curves very quickly approach the $\alpha\Delta\cos\theta$ model. For the $b=0.6$ curve, very little difference can be seen between the layered and $\alpha\Delta\cos\theta$ models. The position of the singularity in this instance will be at twice the maximum gap, which is at $\nu=2\alpha\Delta_0$ in the $\alpha\Delta\cos\theta$ model and at $\nu=2\Delta_0(1+b)$ in the layered model. Such large anisotropy is probably unlikely and hence, in this model, we would expect the region of broadening with softening to be quite narrow. A very interesting point to note is that the gap function does not have to have zeroes in it to exhibit behavior in the phonon self-energy which is d-wave-like.

Finally, in Fig. 6, we present finite-temperature results for this model for a value of the anisotropy $b=0.2$. Again the BCS gap equation [Eq. (3)] has been solved self-consistently for the temperature dependence of the gap. Increasing the anisotropy parameter increasingly reduces the temperature dependence of the gap below that of BCS, but not by very much. Again, as in Fig. 4 for the $\alpha\Delta\cos\theta$ model, we see the curves shift to the left for increasing temperature, tracking the gap as it closes to zero, with the two structures at $2\Delta(T)(1-b)$ and $2\Delta(T)(1+b)$. The overall magnitude also decreases. Measurements of phonon shifts and widths as a function of temperature would effectively map out an image of the basic shape of these curves, as the phonon at different temperatures will resonate with the frequencies of the different features in these curves.

D. Eliashberg strong-coupling calculations

With regard to strong-coupling calculations, the $\alpha\Delta\cos\theta$ and layered superconductor models have been used in a calculation of the phonon self-energy with strong-coupling effects. These results will be reported in detail elsewhere.[29] We mention here that, overall, there is very little difference between the strong-coupling results and the results presented here. The main effect of strong coupling is to produce a reduction in magnitude of the phonon self-energy by a factor of $1+\lambda$, where λ is the electron-boson mass renormalization parameter. This is in agreement with work presented on this point in the

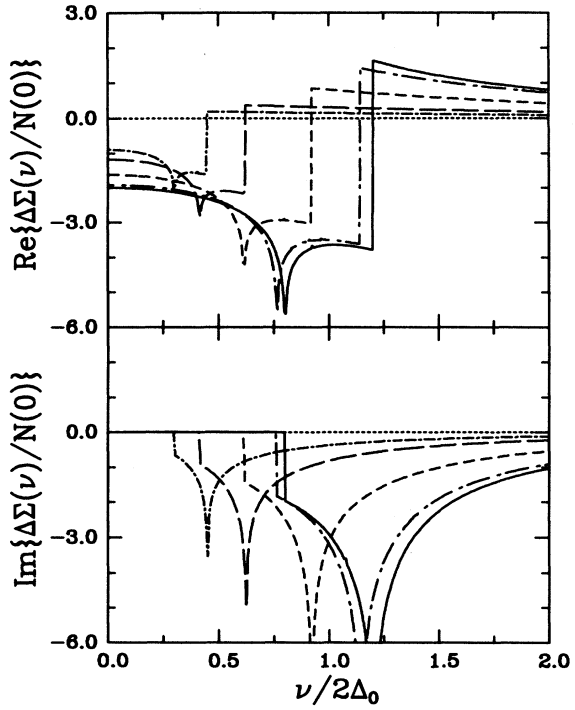

FIG. 6. $\mathbf{q}=0$ phonon self-energy, in BCS theory, at finite temperature and in the clean limit for the case of the $1+b\cos(k_z c)$ model with anisotropy in the electron-phonon coupling $g_{\mathbf{k}} \propto 1+b\cos(k_z c)$. Curves are drawn for $T/T_c=0.0$ (solid curve), 0.6 (dot-long-dashed curve), 0.75 (short-dashed curve), 0.9 (long-dashed curve), and 0.95 (dot-short-dashed curve). Again, negative (positive) values correspond to softening (hardening) in the top frame and broadening (sharpening) in the bottom frame.

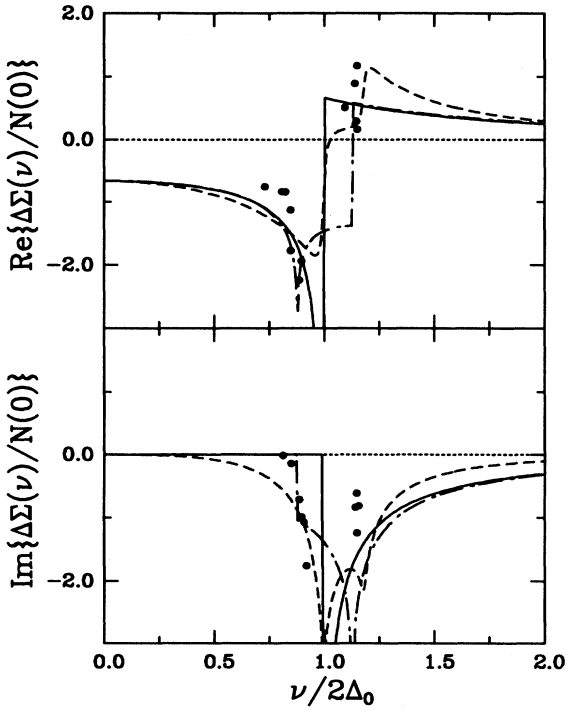

FIG. 7. Comparison between the data of Thomsen *et al.* (Ref. 17) (real part) and Friedl, Thomsen, and Cardona (Ref. 17) (imaginary part) and three models discussed in the text. All models are given in the clean limit. The experimental data has been plotted assuming $2\Delta_0=380$ cm^{-1}. The solid curve is the isotropic s-wave result, the dashed curve is the planar d-wave model (i.e., $\Delta_{\mathbf{k}}=\Delta_0[\cos(k_x a)-\cos(k_y a)]$) for $\bar{\mu}=-0.1$, and the dot-dashed curve is for the layered superconductor model for the anisotropy parameter $b=0.125$. The BCS curves have been scaled by a strong-coupling factor (Ref. 16) corresponding to $\lambda=2$. In the two anisotropic models presented here, the value of $\nu/2\Delta_0=1$ does not simply correspond to twice the energy gap.

context of s-wave pairing by Nicol and Carbotte.[16] If a calculation could be performed for the strong-coupling version of the planar d-wave model of Fig. 1, we would expect to see the second structure due to the van Hove singularity greatly reduced by the strong inelastic scattering.[27,24]

Generally, strong-coupling effects add little to the phonon self-energy other than an overall magnitude change. The phonon self-energy is particularly sensitive to nodes in the gap function with qualitatively different behavior occurring compared with s-wave pairing.

E. Comparison with experiment

Interestingly enough, data have been presented by Thomsen *et al.*[17] for the phonon shifts and by Freidl, Thomsen, and Cardona[17] for the phonon widths, which have been fit to the s-wave theory of Zeyher and Zwicknagl[14] for the real and imaginary parts of the phonon self-energy, respectively. In Fig. 7 we reproduce their data upon which we superimpose curves for three models: isotropic s-wave, planar d-wave, and the layered anisotropic superconductor models, with the parameters given in the figure caption. We have taken $2\Delta_0=380$ cm^{-1} in presenting the data. There are several points to note about this figure: (1) The curves are drawn for the clean limit. Impurity scattering can be expected to round some features and reduce the amount of anisotropy in the d-wave-like models. (2) We have not attempted to find a set of parameters which would best fit the data. (3) Our BCS curves are scaled by a factor of 3, which would correspond to a strong-coupling renormalization parameter λ of 2.[16]

The main conclusion which we draw from this figure is that several different types of models are capable of fitting the data equally well. We cannot say from this figure whether there is d- or s-wave pairing. Certainly, the data for the shifts appear to favor a d-wave interpretation, and this would be consistent with the finite Raman intensity observed in the superconducting state down to zero frequency, below a supposed energy-gap region. In the experimental papers from which the data were taken, fits were made to the Zeyher-Zwicknagl[14] theory with some impurity scattering. The agreement in their case was not

as good for the shifts, but is equally as good for the change in widths.

Finally, in light of this figure, it is not clear what the value of the energy gap might be. For the s-wave curve, the singularity at $\nu/2\Delta_0=1$ corresponds to twice the energy gap; in the planar d-wave model, this point is twice the maximum gap minus a function of the chemical potential, and for the layered superconductor model, the value of $\nu/2\Delta_0=1$ corresponds to the average of the minimum and maximum gaps. While there appears to be support for the existence of a gap, this figure illustrates that it is unclear as to exactly what the gap value might be in this case and which symmetry of the gap function is correct for the high-T_c superconductors.

IV. CONCLUSIONS

We have calculated the $\mathbf{q}=0$ phonon self-energy in the superconducting state for a BCS model where the gap function has d-wave symmetry ($\Delta_{\mathbf{k}}=\Delta[\cos(k_x a)-\cos(k_y a)]$), for a more general model where the gap function has nodes $\Delta_\theta=\alpha\Delta\cos\theta$ and for a model pertinent to layered superconductors with $\Delta_{\mathbf{k}}=\Delta[1+b\cos(k_z c)]$. The d-wave model can be related to the $\alpha\Delta\cos\theta$ model in a constant density-of-states approximation, away from half-filling, and the layered superconductor model can be related to the $\alpha\Delta\cos\theta$ model in the limit of large anisotropy b. In all cases it is found that when the gap parameter has nodes or a constant with a piece with nodes, a phonon has the possibility of being both broadened and softened in the superconducting state, which cannot occur in the clean limit if the gap parameter has pure s-wave symmetry. Therefore experimentally observed broadening with softening could be a signature of a gap parameter exhibiting nodes.

Another possible mechanism which would predict broadening accompanied by softening would be paramagnetic impurity scattering (or a similar pair-breaking mechanism),[30] but the frequency region over which this could occur is expected to be very small for realistic values of the scattering rate.

On a cautionary note, if there exists a van Hove singularity due to two dimensionality, the corresponding structure in the phonon self-energy may be mistakenly identified as the gap singularity. Care must be taken in this regard. Also, the superconducting singularity cannot be identified as twice the energy gap (as in the s-wave case), but is shifted from the maximum d-wave gap by an amount related to the chemical potential, so that once again caution must be exercised in the interpretation of data which might reflect unconventional pairing. We suggest that experiments interpreted within the s-wave model of Zeyher and Zwicknagl[14] could possibly be interpreted with equal success within one of the models presented here. More experiments would have to be done to differentiate between the possibilities, but it would appear that an interpretation that incorporates nodes in the gap function cannot be ruled out at this point.

In conclusion, Raman light-scattering experiments could be a very useful probe of the gap symmetry as in that case there is distinctly different behavior predicted for a gap function with no nodes and one with nodes. This could be used as a test for the high-T_c superconductors and, in principle, for heavy-fermion and organic superconductors, if in the latter case arguments could be found for neglecting vertex corrections to the polarizability.

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