Phonon renormalization and symmetry of the superconducting order parameter

A. Bill
Institut für Physik, Technische Universität Cottbus, P.O. Box 101344, 03013 Cottbus, Germany

V. Hizhnyakov
Tartu University, Tähe 4, Tartu, Estonia

E. Sigmund
Institut für Physik, Technische Universität Cottbus, P.O. Box 101344, 03013 Cottbus, Germany
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We present a method for the calculation of the renormalization of the phonon energy in the superconducting state. The expression is derived in the weak-coupling case and takes into account the **k** dependency of the order parameter $\Delta_{\mathbf{k}}$. The phonon shift as well as the linewidth are calculated. The influence of the anisotropy of the gap in the *ab* plane of the high-T_c superconductors on the renormalization of the $\mathbf{q}\rightarrow 0$ phonon energies is studied. The anisotropies considered have either *s*-, *d*-wave, or mixed character. It is shown that an anisotropic gap with *s*-wave symmetry leads to a renormalization of the phonon energy below T_c that is in agreement with the Raman measurements. The renormalization resulting from the *d*-wave case instead is incompatible with these experiments. Finally, the strength of the electron-phonon coupling is estimated for the Raman observed phonons.

I. INTRODUCTION

Much effort has been devoted in the last years to the experimental determination of the symmetry of the superconducting order parameter in the high-temperature superconductors. Beside the anisotropy between the *ab* plane and the *c* direction, which is a consequence of the anisotropic structure of these materials, a strong deviation from the isotropic case was observed in the *ab* plane itself.[1–6] The question of symmetry, and especially of whether or not there are nodes in the gap or even whether it is a sign alternating function, is important because it could give hints which theory is or is not appropriate in its present form for the description of the high-T_c superconductors. Indeed, some theories predict a symmetry of the gap that has *d*-wave character[7,8] [with nodes along the line $(k_x,\pm k_x,0)$ and change of sign of the function], whereas some other predict an *s*-wave anisotropic gap[9,10] without nodes but still a strong **k** dependence. From the experimental point of view, the situation is not clear. Several experiments, among which were some that were specially designed to solve this problem, suggest that a *d*-wave type gap[1,5,6] and others observe an *s*-wave anisotropy.[3,4]

In the present work we study the influence of the in-plane gap anisotropy on the renormalization of the phonon energy (shift and linewidth) which has a rather anomalous behavior in the high-T_c superconductors. It was observed that one of the Raman lines (340 cm^{-1}) (Refs. 11–13) and the analog IR mode (311 cm^{-1}) (Refs. 14 and 15) show a strong softening in $YBaCu_3O_7$ below the superconducting critical temperature T_c. These modes correspond to the out-of-phase out-of-plane motion of the O(2), O(3) oxygens contained in the Cu_2O planes. Further, the 440-cm^{-1} Raman line (which corresponds to the in-phase out-of-plane motion of the same oxygens) shows a pronounced hardening and broadening in the same temperature region. Replacing Y by other rare-earth elements allowed them to tune experimentally each mode frequency around the value measured for Y and so to study the dependence of the phonon renormalization on its exact position on the energy scale. In every case it was shown[16] that for $T<T_c$ the phonon renormalization disappears when a magnetic field destroying superconductivity is applied to the system. This establishes that the renormalization is directly related to superconductivity.

The theoretical work done up to now to explain the superconductivity-induced renormalization of the phonon energies uses Eliashberg theory. In Ref. 17 an isotropic gap with an account of nonmagnetic impurity scattering was considered, while a *d*-wave-type anisotropy of the order parameter was studied in Ref. 18. The main conclusion of the first work[17] for the present discussion is that in the isotropic case the softening of some of the phonon modes can only be explained under the assumption of a strong electron-phonon coupling and weak impurity scattering rate. The reason is the following. In the weak-coupling case, there is a singularity in the electronic density of states at $\omega=2\Delta$ (where Δ is the BCS gap). Phonons with energy below 2Δ will soften, whereas the other harden. The nearest from the singularity the strongest is the renormalization. When the coupling becomes stronger, the singularity at the gap is damped and shifted to higher energies so that phonon modes which are just above the gap should soften too. The fit of the experiments with the theoretical curves needs a very strong electron-phonon coupling constant ($\lambda\sim 2.9$), which is still an open question and overestimates the

shifts of the phonon energies. Furthermore, it did not take into account the pronounced anisotropy of the gap that was discussed above. The main conclusion of the second work[18] is that a d-wave-type anisotropy of the gap allows a better explanation of the available experimental data for the shift of the phonons than the pure isotropic (s-wave) case.

In the following we present a method to calculate the superconductivity-induced shift and linewidth of any phonon mode and any wave vector $\mathbf{q}$ in the weak-coupling limit (Sec. II). The wave-vector dependence of the superconducting order parameter is thereby explicitly taken into account. For $\mathbf{q}=0$ phonons the result coincides with that given in Ref. 18. With the expression obtained for the shift and linewidth of the phonon lines, we calculate in Sec. III the renormalization of the Raman and IR-active modes considering a simple model for the pairing potential in the layered structures. We can then study the influence of several types of anisotropies on the renormalization and draw some conclusions about the compatibility of the obtained curves with the experiments. One of the main conclusions of the numerical part of the calculations is that a d-wave anisotropy of the gap leads to a renormalization of the phonons that is in contradiction with the observed behavior of the Raman and IR linewidths, whereas the anisotropic s-wave case can be fitted in a semiquantitative way for both the shift and the linewidth of the phonon line. We find furthermore that the strength of the electron-phonon coupling for each mode observed by Raman spectroscopy is rather small (~ 0.01 eV), although the total coupling is moderate (~ 0.1 eV).

The method presented in the next section not only gives the renormalization of the phonons for any wave vector, but also a set of self-consistent equations for the Hartree-Fock mean field, the gap function, and the renormalization of the electron-lattice interaction in the superconducting state. The equations for the gap that are explicitly derived can be considered as the $\mathbf{k}$-dependent analog of the Eliashberg equations.

II. PHONON RENORMALIZATION

The system (superconductor) is described by the Hamiltonian

$$H = H_e + H_L + H_{eL} \ , \tag{1}$$

where

$$H_e = \sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} \tag{2}$$

is the Hamiltonian of the charge carriers (electrons, holes), $c^{\dagger}_{\mathbf{k},\sigma}$ ($c_{\mathbf{k},\sigma}$) is the creation (destruction) operator of the particle with wave vector $\mathbf{k}$ and spin index σ (which has the values $\uparrow$ and $\downarrow$),

$$H_L = \sum_{\mathbf{q},\nu} \hbar\omega_{\nu\mathbf{q}} (b^{\dagger}_{\nu\mathbf{q}} b_{\nu\mathbf{q}} + \tfrac{1}{2}) \tag{3}$$

is the Hamiltonian of the lattice vibrations, $b^{\dagger}_{\nu\mathbf{q}}$ ($b_{\nu\mathbf{q}}$) is the creation (destruction) operator of the phonon of branch ν, wave vector $\mathbf{q}$, and frequency $\omega_{\nu\mathbf{q}}$, and

$$H_{eL} = \sum_{\mathbf{k},\mathbf{q}} \sum_{\sigma,\nu} g_{\nu}(\mathbf{q}) c^{\dagger}_{\mathbf{k},\sigma} c_{\mathbf{k}+\mathbf{q},\sigma} b^{\dagger}_{\nu\mathbf{q}} + \text{H.c.} \tag{4}$$

is the electron-lattice interaction which is linear in the phonon operators. $g_{\nu}(\mathbf{q})$ is the interaction function assumed here to be only dependent on $\mathbf{q}$. We further consider only one conducting band but all phonon branches. These two restrictions, however, are not fundamental for the calculations.[19] The two first terms of the Hamiltonian are usually considered as the zero-order Hamiltonian and the third as the perturbation of the charge-carrier–phonon system.

To describe the experimentally observed influence of superconductivity onto the Raman and IR-active phonons, we have to include in the zeroth order of the Hamiltonian the appearance of the gap in the electronic spectrum.[20] To this aim we add and subtract to H the following terms:

$$H_{\phi} = \sum_{\mathbf{k}} \phi_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\uparrow} c^{\dagger}_{-\mathbf{k}\downarrow} + \text{H.c.} \ , \tag{5}$$

$$H_{\chi} = \sum_{\mathbf{k},\sigma} \chi_{\mathbf{k}} c^{\dagger}_{\mathbf{k},\sigma} c_{\mathbf{k}\sigma} \ , \tag{6}$$

$$\delta H_L = \sum_{\mathbf{q},\nu} \delta\omega_{\nu\mathbf{q}} b^{\dagger}_{\nu\mathbf{q}} b_{\nu\mathbf{q}} \ , \tag{7}$$

$$\delta H_{eL} = \sum_{\mathbf{k},\sigma} \sum_{\nu\mathbf{q}} \delta g_{\nu}(\mathbf{q}) c^{\dagger}_{\mathbf{k},\sigma} c_{\mathbf{k}+\mathbf{q},\sigma} b^{\dagger}_{\nu\mathbf{q}} + \text{H.c.} \tag{8}$$

The first two terms describe the superconducting (gap) and Hartree-Fock mean fields. The two next terms describe the renormalization of the phonon energy and of the electron-phonon interaction. They are assumed to be second-order effects and can be considered as small. The new zero-order Hamiltonian can now be defined as

$$H_0 = H_{\text{SC}} + \bar{H}_L \ , \tag{9}$$

where

$$\begin{aligned} H_{\text{SC}} &= H_e + H_{\phi} + H_{\chi} - \mu N \\ &= \sum_{\mathbf{k}} E_{\mathbf{k}} (a^{\dagger}_{1\mathbf{k}} a_{1\mathbf{k}} + a^{\dagger}_{2\mathbf{k}} a_{2\mathbf{k}}) \end{aligned} \tag{10}$$

and $\bar{H}_L = H_L + \delta H_L$ is the renormalized phonon Hamiltonian. The electronic part H_{SC} is diagonalized using the Bogoliubov transformation

$$a_{1\mathbf{k}} = u_{\mathbf{k}} c_{\mathbf{k}\uparrow} + v_{\mathbf{k}} c^{\dagger}_{-\mathbf{k}\downarrow} \ ,$$

$$a_{2\mathbf{k}} = v_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\uparrow} - u_{\mathbf{k}} c_{-\mathbf{k}\downarrow} \ ,$$

with

$$u_{\mathbf{k}} = \sqrt{\tfrac{1}{2}(1 + \bar{\varepsilon}_{\mathbf{k}}/E_{\mathbf{k}})}, \quad v_{\mathbf{k}} = \sqrt{\tfrac{1}{2}(1 - \bar{\varepsilon}_{\mathbf{k}}/E_{\mathbf{k}})} \ .$$

$u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ are chosen real to simplify the notation. The energy of the one-particle excitation is given by

$$E_{\mathbf{k}} = \sqrt{\bar{\varepsilon}^2_{\mathbf{k}} + \Delta^2_{\mathbf{k}}} \ , \tag{11}$$

with $\bar{\varepsilon}_{\mathbf{k}} = \varepsilon_{\mathbf{k}} - \chi_{\mathbf{k}} - \mu$. $\Delta_{\mathbf{k}} = |\phi_{\mathbf{k}}|$ is the gap parameter. To keep the following algebra as simple as possible, we neglect here the phase of the gap, but the final expressions will contain it. Finally, N is the particle number

operator and μ is the chemical potential, which can be found by standard methods (see, e.g., Ref. 21).

The total Hamiltonian takes the form

$$H=H_0+H' , \tag{12}$$

$$H'=\bar{H}_{eL}-H_\phi-H_\chi-\delta H_L-\delta H_{eL} , \tag{13}$$

where $\bar{H}_{eL}=H_{eL}+\delta H_{eL}$. The unknown functions $\phi_{\mathbf{k}}$, $\chi_{\mathbf{k}}$, $\delta\omega_{\nu\mathbf{q}}$, and $\delta g_\nu(\mathbf{q})$ have to be determined in a self-consistent way. We can outline the idea of the procedure for the calculation of these parameters as follows. Since the new zero-order Hamiltonian describes the system in the superconducting state, we have to remove the linear renormalized electron-phonon coupling $\bar{H}_{eL}$. This will be done in first order by applying a unitary transformation to Eq. (12). The transformed Hamiltonian considered up to second order in the renormalized electron-phonon coupling constant contains H_0 and residual terms arising from the application of the transformation. In a second step we require that these terms taken in the mean-field approximation give no contribution to the electron and phonon self-energies in lowest order. In this way one obtains a set of nonlinear equations for the gap $\Delta_{\mathbf{k}}$, the Hartree-Fock mean field $\chi_{\mathbf{k}}$, and the interaction constant $\delta g_\nu(\mathbf{q})$ as well as an expression for the renormalization of the phonon energy. Since we are here mainly concerned with the determination of the last parameter, we will only briefly sketch the derivation of the equations for $\Delta_{\mathbf{k}}$, $\chi_{\mathbf{k}}$, and $\delta g_\nu(\mathbf{q})$.

We apply onto Eq. (12) a unitary transformation expressed in exponential form as $U=e^{-S}$ with

$$S=\sum_{\mathbf{k},\mathbf{q}}\sum_{\nu}\bar{g}_\nu(\mathbf{q})(\alpha_1 a^\dagger_{1\mathbf{k}}a_{1\mathbf{k}+\mathbf{q}}+\alpha_2 a^\dagger_{2\mathbf{k}+\mathbf{q}}a_{2\mathbf{k}} +\alpha_3 a^\dagger_{1\mathbf{k}}a^\dagger_{2\mathbf{k}+\mathbf{q}}+\alpha_4 a_{2\mathbf{k}}a_{1\mathbf{k}+\mathbf{q}})b^\dagger_{\nu\mathbf{q}}-\text{H.c.} \tag{14}$$

$[\bar{g}_\nu(\mathbf{q})=g_\nu(\mathbf{q})+\delta g_\nu(\mathbf{q})]$. The functions α_1–α_4 are defined by the condition

$$[S,H_0]=-\bar{H}_{eL} \tag{15}$$

and given by

$$\alpha_1=\frac{\beta}{E_{\mathbf{k}}-E_{\mathbf{k}+q}+\hbar\omega_{\nu\mathbf{q}}},\quad \alpha_2=-\frac{\beta}{E_{\mathbf{k}}-E_{\mathbf{k}+\mathbf{q}}-\hbar\omega_{\nu\mathbf{q}}} ,$$

$$\alpha_3=\frac{\beta}{E_{\mathbf{k}}+E_{\mathbf{k}+\mathbf{q}}+\hbar\omega_{\nu\mathbf{q}}},\quad \alpha_4=-\frac{\beta'}{E_{\mathbf{k}}+E_{\mathbf{k}+\mathbf{q}}-\hbar\omega_{\nu\mathbf{q}}} , \tag{16}$$

$$\beta=u_{\mathbf{k}}u_{\mathbf{k}+\mathbf{q}}-v_{\mathbf{k}}v_{\mathbf{k}+\mathbf{q}},\quad \beta'=u_{\mathbf{k}}v_{\mathbf{k}+\mathbf{q}}+u_{\mathbf{k}+\mathbf{q}}v_{\mathbf{k}} .$$

Here we use the notation $\alpha_i\equiv\alpha_i(\mathbf{k},\nu\mathbf{q})$, $\beta^{(\prime)}\equiv\beta^{(\prime)}(\mathbf{k},\mathbf{q})$. Since the zero-order Hamiltonian H_0 is diagonal in the Bogoliubov operators, it is best to express every term in these operators. The electron-phonon interaction takes the form

$$\bar{H}_{eL}=\sum_{\mathbf{k}}\sum_{\mathbf{q}\nu}\bar{g}_\nu(\mathbf{q})[\beta(a^\dagger_{1\mathbf{k}}a_{1\mathbf{k}+\mathbf{q}}+a^\dagger_{2\mathbf{k}+\mathbf{q}}a_{2\mathbf{k}}) +\beta'(a^\dagger_{1\mathbf{k}}a^\dagger_{2\mathbf{k}+\mathbf{q}}+a_{2\mathbf{k}}a_{1\mathbf{k}+\mathbf{q}})]b^\dagger_{\nu\mathbf{q}}+\text{H.c.} , \tag{17}$$

and for the electronic renormalization one has

$$H_\Delta+H_\chi=\sum_{\mathbf{k}}E_{\mathbf{k}}^{-1}[(\chi_{\mathbf{k}}\bar{\varepsilon}_{\mathbf{k}}+\Delta_{\mathbf{k}}^2)(a^\dagger_{1\mathbf{k}}a_{1\mathbf{k}}+a^\dagger_{2\mathbf{k}}a_{2\mathbf{k}}) +(\chi_{\mathbf{k}}-\bar{\varepsilon}_{\mathbf{k}})\Delta_{\mathbf{k}}(a^\dagger_{1\mathbf{k}}a^\dagger_{2\mathbf{k}}+a_{2\mathbf{k}}a_{1\mathbf{k}})] . \tag{18}$$

Assuming a weak coupling between the charge carriers and the phonon system, we perform the transformation up to second order of the renormalized coupling constant and obtain

$$\tilde{H}=H_0+\tilde{H}'+\tilde{H}'' , \tag{19}$$

with

$$\tilde{H}'=\tfrac{1}{2}[S,\bar{H}_{eL}]-H_\Delta-H_\chi-\delta H_L , \tag{20}$$

$$\tilde{H}''=-\delta H_{eL}-[S,H_\Delta+H_\chi]-\tfrac{1}{2}[S,[S,H_\Delta+H_\chi]] . \tag{21}$$

For the following we only need to calculate explicitly the commutator included in $\tilde{H}'$. One obtains

$$\tfrac{1}{2}[S,\bar{H}_{eL}]_{ee}=\sum_{\mathbf{k}}\sum_{\mathbf{q}\nu}|\bar{g}_\nu(\mathbf{q})|^2 \times[\alpha(a^\dagger_{1\mathbf{k}}a_{1\mathbf{k}+\mathbf{q}}+a^\dagger_{2\mathbf{k}+\mathbf{q}}a_{2\mathbf{k}})+\alpha'(a^\dagger_{1\mathbf{k}}a^\dagger_{2\mathbf{k}+\mathbf{q}}+a_{2\mathbf{k}}a_{1\mathbf{k}+\mathbf{q}})] \times[\beta(a^\dagger_{1\mathbf{k}+\mathbf{q}}a_{1\mathbf{k}}+a^\dagger_{2\mathbf{k}}a_{2\mathbf{k}+\mathbf{q}})+\beta'(a^\dagger_{1\mathbf{k}+\mathbf{q}}a^\dagger_{2\mathbf{k}}+a_{2\mathbf{k}+\mathbf{q}}a_{1\mathbf{k}})] , \tag{22}$$

$$\tfrac{1}{2}[S,\bar{H}_{eL}]_{eL}=\sum_{\mathbf{q}\nu}\left\{\sum_{\mathbf{k}}[|\bar{g}_\nu(\mathbf{q})|^2\bar{\alpha}\beta(a^\dagger_{1\mathbf{k}}a_{1\mathbf{k}}+a^\dagger_{2\mathbf{k}}a_{2\mathbf{k}})+\bar{\alpha}'\beta'(a^\dagger_{1\mathbf{k}}a_{1\mathbf{k}}+a^\dagger_{2\mathbf{k}}a_{2\mathbf{k}}-1) +(\bar{\alpha}\beta'+\bar{\alpha}'\beta)(a^\dagger_{1\mathbf{k}}a^\dagger_{2\mathbf{k}}+a_{2\mathbf{k}}a_{1\mathbf{k}})]\right\}b^\dagger_{\nu\mathbf{q}}b_{\nu\mathbf{q}} , \tag{23}$$

where

$$\alpha=\tfrac{1}{2}(\alpha_1+\alpha_2),\quad \bar{\alpha}=\tfrac{1}{2}(\alpha_1-\alpha_2) ,$$
$$\alpha'=\tfrac{1}{2}(\alpha_3+\alpha_4),\quad \bar{\alpha}'=\tfrac{1}{2}(\alpha_3-\alpha_4) , \tag{24}$$

Here we neglect terms with $\mathbf{k}\neq\mathbf{k}'$ and $\mathbf{q}\neq\mathbf{q}'$ as well as terms $\sim b^\dagger_{\nu\mathbf{q}}b^\dagger_{\nu\mathbf{q}}$ and $b_{\nu\mathbf{q}}b_{\nu\mathbf{q}}$ because in the present calculation these expressions will contribute to the two-particle interaction and to the phonon renormalization only in higher order. The first commutator is a two-particle in-

teraction, whereas the second is a nonlinear electron-phonon interaction that will give rise to an effective phonon renormalization in the mean field.

The parameters in Eqs. (5)–(8) are now determined in such a way that the contributions of $\tilde{H}'+\tilde{H}''$ to the electron and phonon self-energies vanish in the mean-field approximation. In this approximation one replaces the operators $a_{i\mathbf{k}}^{\dagger}a_{i\mathbf{k}}$ ($i=1,2$) by the mean fields

$$\langle a_{i\mathbf{k}}^{\dagger}a_{i\mathbf{k}}\rangle \equiv f_{\mathbf{k}}=(e^{\beta E_{\mathbf{k}}}+1)^{-1} ,$$
$$\langle a_{i\mathbf{k}}^{\dagger}a_{i\mathbf{k}}^{\dagger}\rangle=\langle a_{i\mathbf{k}}a_{i\mathbf{k}}\rangle=0 \quad \text{for } i=1,2 . \tag{25}$$

$\Delta_{\mathbf{k}}$ and $\chi_{\mathbf{k}}$ are then determined by the condition

$$\Sigma(\tfrac{1}{2}\langle [S,\bar{H}_{eL}]_{ee}\rangle)=\Sigma(H_{\phi}+H_{\chi}) ,$$

where the commutator is given by Eq. (22) and Σ is the electron self-energy part coming from the operator in parentheses. This leads to the equations

$$\chi_{\mathbf{k}}\bar{\varepsilon}_{\mathbf{k}}+\Delta_{\mathbf{k}}^2=E_{\mathbf{k}}\sum_{\nu\mathbf{q}}|\bar{g}_{\nu}(\mathbf{q})|^2(1-2f_{\mathbf{k}+\mathbf{q}})(\alpha\beta-\alpha'\beta') ,$$
$$\Delta_{\mathbf{k}}(\chi_{\mathbf{k}}-\bar{\varepsilon}_{\mathbf{k}})=E_{\mathbf{k}}\sum_{\nu\mathbf{q}}|\bar{g}_{\nu}(\mathbf{q})|^2(1-2f_{\mathbf{k}+\mathbf{q}})(\alpha'\beta+\alpha\beta') . \tag{26}$$

They can be considered as a version of the Eliashberg equations with an explicit account of the wave-vector dependence of the superconducting parameters. The BCS gap equation is a special case of Eq. (26) when $\bar{\varepsilon}_{\mathbf{k}}=0$. In the numerical part we will take this special case for the calculation of the gap. The condition giving the renormalization of the electron-phonon coupling constant is

$$\Pi(\delta H_{eL}+[S,H_{\phi}+H_{\chi}]+\tfrac{1}{2}\langle [S[S,H_{\phi}+H_{\chi}]]\rangle)=0 ,$$

where Π is the phonon self-energy (polarization). The equation for this parameter is rather lengthy. Since we do not need the exact expression of $\delta g_{\nu}(\mathbf{q})$ for the numerical calculations of the next section, we do not consider it. The last parameter that is to be calculated is the renormalization of the phonon energy. The condition determining this quantity is

$$\Pi(\delta H_L)=\Pi(\tfrac{1}{2}\langle [S,\bar{H}_{eL}]_{eL}\rangle) . \tag{27}$$

The commutator is given by Eq. (23). The calculation is straightforward, and one obtains

$$\delta\omega_{\nu\mathbf{q}}=|\bar{g}_{\nu}(\mathbf{q})|^2\sum_{\mathbf{k}}\left[\frac{\bar{f}_{\mathbf{k}}(E_{\mathbf{k}+\mathbf{q}}-E_{\mathbf{k}})(E_{\mathbf{k}}E_{\mathbf{k}+\mathbf{q}}+\bar{\varepsilon}_{\mathbf{k}}\varepsilon_{\mathbf{k}+\mathbf{q}}-\Delta_{\mathbf{k}}\Delta_{\mathbf{k}+\mathbf{q}})}{E_{\mathbf{k}}E_{\mathbf{k}+\mathbf{q}}[(\hbar\omega_{\nu\mathbf{q}})^2-(E_{\mathbf{k}}-E_{\mathbf{k}+\mathbf{q}})^2]}\right.$$
$$\left.+\frac{(1-2\bar{f}_{\mathbf{k}})(E_{\mathbf{k}+\mathbf{q}}+E_{\mathbf{k}})(E_{\mathbf{k}}E_{\mathbf{k}+\mathbf{q}}-\bar{\varepsilon}_{\mathbf{k}}\bar{\varepsilon}_{\mathbf{k}+\mathbf{q}}+\Delta_{\mathbf{k}}\Delta_{\mathbf{k}+\mathbf{q}})}{E_{\mathbf{k}}E_{\mathbf{k}+\mathbf{q}}[(\hbar\omega_{\nu\mathbf{q}})^2-(E_{\mathbf{k}}+E_{\mathbf{k}+\mathbf{q}})^2]}\right] . \tag{28}$$

This expression gives the superconductivity-induced renormalization of the energy of the phonon mode ν with wave vector $\mathbf{q}$ for the weak-coupling case. As already supposed, it is a second-order effect in the electron-phonon coupling constant. Taking into account the phase φ of the gap ($\phi_{\mathbf{k}}=\Delta_{\mathbf{k}}e^{i\varphi_{\mathbf{k}}}$), only the product $\Delta_{\mathbf{k}}\Delta_{\mathbf{k}+\mathbf{q}}$ changes to $\Delta_{\mathbf{k}}\Delta_{\mathbf{k}+\mathbf{q}}\cos(\varphi_{\mathbf{k}}-\varphi_{\mathbf{k}+\mathbf{q}})$. The main experimental work done until now was to determine the phonon renormalization of the Raman and IR-active modes that are measured at $\mathbf{q}\sim 0$. In this case Eq. (28) takes the simple form

$$\delta\omega_{\nu 0}=-4|\bar{g}_{\nu}(0)|^2\sum_{\mathbf{k}}\frac{\Delta_{\mathbf{k}}^2(1-2\bar{f}_{\mathbf{k}})}{E_{\mathbf{k}}[(2E_{\mathbf{k}})^2-(\hbar\omega_{\nu 0})^2]} . \tag{29}$$

This result agrees with Ref. 18. The $\mathbf{k}$ dependence of the order parameter is here explicitly taken into account. This allows one to study the influence of the anisotropy of the gap on the renormalization of the phonon energy. This will be done for a simple model in the next section. It should be mentioned that an analogous study was performed in Ref. 18; however, they did not consider the s-wave anisotropic case and obtained conclusions that differ from those presented below.

The unitary transformation used in the present calculation is not the only one that removes the electron-phonon interaction in first order as was shown in Refs. 19, 20, and 22. The two-step transformation, which is especially interesting when considering nontotally screened long-range electron-phonon couplings as well as the distortive electron-lattice interaction in the high-T_c superconductors, gave, however, exactly the same expression as Eq. (29). Furthermore, the calculations were here performed for the case of one electronic band for simplicity, but the generalization to several bands is straightforward. We note that although expressions (28) and (29) have been derived here for Cooper pairing caused only by electron-phonon interaction, an account of other pairing mechanisms (which can be performed in a straightforward way by including additional H_{ϕ}- and H_{χ}-type terms into H) is also possible.

III. NUMERICAL RESULTS

For the numerical calculation of the renormalization of the $\mathbf{q}=0$ phonons, we have to take correctly into account the poles of the integrand of Eq. (29). Following the procedure used in the Green function technique, we replace

the energy $\omega_{\nu 0}$ in the denominator of Eq. (29) by a complex one $\omega_{\nu 0} \rightarrow \omega_{\nu 0} - i\eta$ so that the phonon Green function is properly defined. η is an infinitesimal real positive quantity. This extension to the complex plane could also have been done from the beginning by replacing $\omega_{\nu \mathbf{q}}$ in the unitary transformation (14) by a complex frequency. As a result, one obtains the complex phonon frequency renormalization $\delta\omega_{\nu 0} = \Delta\omega_{\nu 0} + i\Delta\gamma_{\nu 0}$, which corresponds to the shift $\Delta\omega_{\nu 0}$ and the change of the linewidth, $\Delta\gamma_{\nu 0}$, of the phonon line due to the damping of phonons by breaking Cooper pairs. One then obtains (in the limit $\eta \rightarrow 0$ and continuous $\mathbf{k}$)

$$\Delta\omega_{\nu 0} = -|\bar{g}_{\nu}(0)|^2 P \int \frac{d\mathbf{k}}{\pi^3} \frac{\Delta_{\mathbf{k}}^2 D_{\mathbf{k}}}{(2E_{\mathbf{k}})^2 - \omega_{\nu 0}^2} , \tag{30}$$

$$\Delta\gamma_{\nu 0} = \pi |\bar{g}_{\nu}(0)|^2 \int \frac{d\mathbf{k}}{\pi^3} \delta(4E_{\mathbf{k}}^2 - \omega_{\nu 0}^2) \Delta_{\mathbf{k}}^2 D_{\mathbf{k}} , \tag{31}$$

where P indicates that the principal value of the integral has to be taken. $D_{\mathbf{k}}$ is defined in Eq. (32) below. In the following we calculate the sum of these expressions as a function of ω and always normalize the shift and linewidth to $|\bar{g}_{\nu}(0)|^2$. To obtain the curves shown in the following figures, we replaced $\omega_{\nu 0}$ under the integrals in Eqs. (30) and (31) by a continuous energy variable ω. The renormalization of a specific phonon is then obtained for $\omega = \omega_{\nu 0}$. $\Delta\omega_{\nu 0} < 0$ corresponds to a softening of the phonon, and $\Delta\gamma_{\nu 0} > 0$ gives the broadening of the phonon line.

The gap equation used for the numerical calculations is of BCS type, which is a special case of Eq. (26) as already mentioned. Setting $\chi_{\mathbf{k}} \equiv 0$, one has

$$\Delta_{\mathbf{k}} = -\sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} \Delta_{\mathbf{k}'} D_{\mathbf{k}'} \quad \text{with } D_{\mathbf{k}} = \frac{\tanh(\beta E_{\mathbf{k}}/2)}{2E_{\mathbf{k}}} . \tag{32}$$

The model we consider in the following takes into account the essential features of the layered structure of the high-T_c materials that are needed for the present discussion.[23-25] The electronic normal-state energy spectrum, Eq. (2), is described by one band taking into account nearest- (t) and next-nearest- (t_1) neighbor intralayer and interlayer (t_2) hopping to fit correctly the band structure calculations for the $YBa_2Cu_3O_{7-\delta}$ system,[26]

$$\varepsilon_{\mathbf{k}} = t\{2[\cos(k_x a) + \cos(k_y a)] - 4t_1 \cos(k_x a)\cos(k_y a) + 2t_2(\cos(k_x c) + \mu'\} . \tag{33}$$

The parameters are set to $t = -0.25$ eV, $t_1 = 0.45$, and $t_2 = 0.1$.[9,24] The energies are scaled to the nearest-neighbor transfer integral energy t. We have assumed that the in-plane lattice constants along the a and b axes are equal [in the following we replace $(k_{x,y}a)$ by $k_{x,y}$]. The pairing potential considered is a nonseparable, nonretarded (without cutoff) interaction between nearest neighbors within the planes

$$V_{\mathbf{k}\mathbf{k}'} = V_0 + V_1[\cos(k_x - k_x') + \cos(k_y - k_y')] . \tag{34}$$

In Sec. III C we add an interplanar pairing to (34) and discuss its influence on the phonon renormalization. It is clear that this simple model cannot account for all the properties of the high-T_c superconductors. Especially, the electronic phase separation (Ref. 27, and references therein) which appears in these systems at relatively low doping rates is not taken into account, although this fact may be important in the determination of the anisotropy of the gap.

The chosen shape (34) of the interaction implies that the solutions of Eq. (32) have the form $\Delta_{\mathbf{k}} = \Delta_0 + \Delta_x \cos(k_x) + \Delta_y \cos(k_y)$. Depending on the value of the chemical potential $\mu = t\mu'$ and the temperature T, the solution will have either s-wave isotropic ($\Delta_0 \neq 0$, $\Delta_x = \Delta_y = 0$), s-wave anisotropic ($\Delta_x = \Delta_y \neq 0$), d-wave ($\Delta_0 = 0$, $\Delta_x = -\Delta_y \neq 0$), or mixed ($\Delta_0 \neq 0 \neq \Delta_x \neq \Delta_y$) character. A general study of the possible solutions of the gap equation for the model Eq. (34) was done with the help of bifurcation theory.[25] We could infer from it that for our band structure parameters in the case $V_0 = 0$ at $T = 0$ one finds an s-wave anisotropic solution for $\mu' \lesssim -2.1$, a mixed solution for $-2.1 \lesssim \mu' \lesssim -1.8$, and a d-wave solution for $\mu' \gtrsim -1.8$. To ensure that we have the right solution for each parameter set (especially when $\Delta_0 \neq 0$), we calculated the Gibbs free energy (according to Ref. 25), which must be the lowest for the stable solution. In the following we exclusively consider these stable solutions of the gap equa-

TABLE I. Values of the parameters and of the gap used for the calculations of the phonon renormalization. All energies are given in meV. T_c is 90 K in every case.

V_0	V_1	V_z	Δ_0	Δ_x	Δ_y	Δ_z	$\Delta_{\max}$	T/T_C
s wave ($\mu' = -2.22$)								
−248	0	0	13.7	0	0	0	13.7	0
−150	−150	0	7.0	4.4	Δ_x	0	15.8	0
0	−299	0	0	8.5	Δ_x	0	17.0	0
0	−299	0	0	5.6	Δ_x	0		0.83
0	−299	0	0	2.0	Δ_x	0		0.98
−247	0	−9.0	14.1	0	Δ_x	1.6	15.7	0
0	−290	−7.0	0	8.0	Δx	0.9	16.9	0
d wave ($\mu' = -1.35$)								
0	−299	0	0	8.8	$-\Delta_x$	0	17.6	0
0	−299	0	0	5.6	$-\Delta_x$	0		0.83
0	−299	0	0	1.9	$-\Delta_x$	0		0.98

tion. One should mention at this point that many physical quantities were calculated in the framework of this model in Ref. 24 (and references therein). Here we merely use the model as a tool to study the influence of the anisotropy of the gap onto the phonon renormalization. The main conclusions are not dependent on the special features of the model as was shown in Refs. 19 and 28.

In Table I we summarize the stable solutions of Eq. (32) used to calculate the phonon shift and linewidths. The parameters V_0, V_1, and V_x for the pairing potential were always chosen in such a way that the critical temperature is $T_C(\mu)=90$ K. We fixed the value $\mu'=-1.35$ (in this case the solution has d-wave symmetry) because the Fermi surface then reproduces the one obtained in band structure calculations for $YBaCu_3O_7$ (Refs. 7 and 26) [for $\mu'\leq -2$ the Fermi surface is closed around the Γ point of the Brillouin zone, whereas in the other case it is open and looks like a corrugated cylinder along the line (π,π,k_x)]. For the s-wave solution we chose $\mu'\simeq -2.22$ because for the same parameters as the d-wave case one obtains again $T_c=90$ K [we recall that the function $T_C(\mu')$ is zero below $\mu'=-2.42$, goes through a maximum at $\mu'\simeq -1.8$, and then vanishes toward $\mu'=0$]. We have now all the ingredients necessary to calculate the phonon renormalization. Since the change of μ' with temperature was shown to be very small and without consequence for the following discussions, we kept it at the $T=0$ value for the temperature-dependent calculations.

A. s-wave anisotropy

In Figs. 1 and 2 we show the phonon shift and linewidth, respectively, for different s-wave anisotropies. All were considered for $\mu'\simeq -2.22$. They show how the renormalization changes when the gap goes from a constant value ($\Delta_0\neq 0$, $\Delta_x=\Delta_y=0$) to a pure anisotropic s-wave solution ($\Delta_0=0$, $\Delta_y\neq 0$).

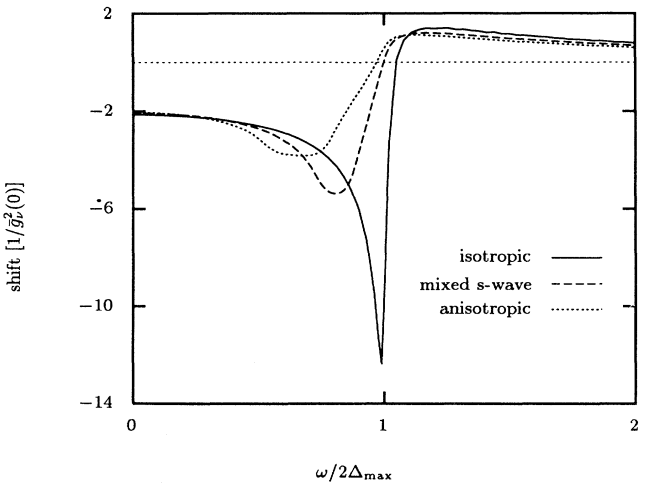

FIG. 1. Real part of $\delta\omega_{v0}$ for the s-wave case at $T=0$. $V_0=-0.248$, $V_1=0$ (solid line); $V_0=V_1=-0.15$ (dashed line); $V_0=0$, $V_1=-0.299$ (dotted line). V_0, V_1 in eV. $\mu'\simeq -2.22$. Δ_{max} has a different value for each curve.

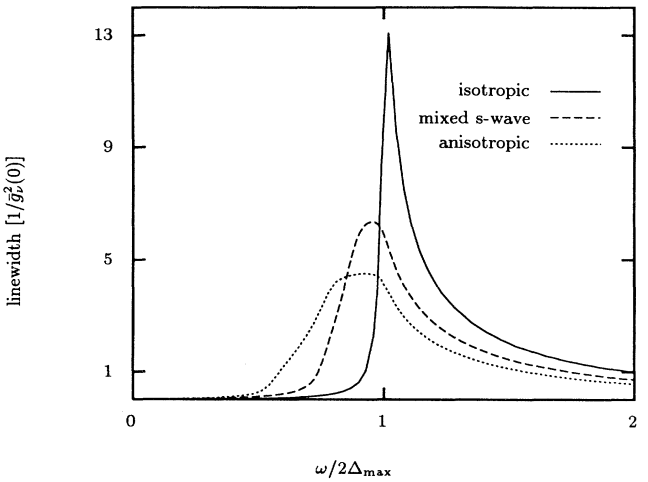

FIG. 2. Imaginary part of $\delta\omega_{v0}$ for the s-wave case at $T=0$. $V_0=-0.248$, $V_1=0$ (solid line); $V_0=V_1=-0.15$ (dashed line); $V_0=0$, $V_1=-0.299$ (dotted line). V_0, V_1 in eV. $\mu'\simeq -2.22$. Δ_{max} has a different value for each curve.

The BCS case can be calculated analytically[17] and shows a singularity at the energy $\omega=2\Delta_{max}=2\Delta$. Phonons with energy below this value soften and those above harden. Further, the linewidth is zero below 2Δ, whereas it slowly goes to zero from above for increasing energy above the singularity. The value of (30) at $\omega=0$ for the BCS case is given by $-2N(0)\omega_c/\sqrt{\omega_c^2+\Delta^2}$. $N(0)$ is the density of states at the Fermi energy in the normal phase, and ω_c is the cutoff of the potential which is a characteristic phonon energy. The solid curves in Figs. 1 and 2 correspond to an extension of the BCS case since they are obtained for a constant potential without an energy cutoff. The main difference with the BCS case is that lifetime effects damp the singularity. Otherwise, the curves are rather similar. The dotted line shows the case of a pure s-wave anisotropic gap. There are some important differences between these curves and the pure BCS result (or its extension, solid line), which we discuss in the following. First, the singularity in Fig. 1 is rather strongly damped and the curve about the minima is broaden. This property is also reflected in Fig. 2 where the curve no longer falls abruptly from zero to the minimum. Second, the jump from negative to positive values of $\Delta\omega_{v0}$ becomes a smooth transition for an s-wave anisotropic gap. These effects are related to the fact that the gap anisotropy washes out the singularity of the electronic density of states (DOS) for energies above the gap. For a constant gap (BCS case), the DOS is zero in the gap region. At the upper edge of the gap, the DOS has a singularity and falls down as $\varepsilon/\sqrt{\varepsilon^2-\Delta^2}$ for higher energies. Because of the gap anisotropy, electronic states are located between $2\Delta_{max}$ and $2\Delta_{min}$. Phonons with energy in this region have thus sufficient energy to break Cooper pairs. The third difference compared to the BCS case is that the minimum is shifted to lower energies. This reflects the

fact that in the present calculations the minimum of the gap is getting smaller with the increase of V_1 and the simultaneous decrease of V_0. The next difference which follows from the discussion about the electronic DOS is that the superconductivity-induced softening of the phonons is not limited to energies below the gap. This is thus not an exclusive property of the strong-coupling limit.[17] The softening is here, however, still restricted to energies below the maximum of the gap. The fifth distinctive feature of the dotted curve compared to the pure BCS case is that there is still a value of the energy below which the change of the linewidth is vanishing as in the case for an isotropic gap. The last difference to mention here is that the value at $\omega=0$ diminishes with increasing anisotropy, although only for a small amount. The dashed curve in Figs. 1 and 2 shows an intermediate case between an isotropic and a pure s-wave anisotropic gap. It demonstrates that when increasing the anisotropic part V_1 with respect to V_0 in Eq. (34) the change between the two discussed limiting cases (solid and dotted lines) is continuous. In Figs. 3 and 4 we show the temperature dependence of the shift and linewidth, respectively, for the pure s-wave anisotropic case (dotted line in Figs. 1 and 2). As one can see, the behavior of these curves does not change drastically from the BCS case. When the temperature increases the whole curve shifts to smaller energies, reflecting the decrease of the gap with temperature. Moreover, the minimum tends toward zero when $T\rightarrow T_c$. As a consequence, a phonon with energy well above (below) the maximum of the gap will always experience a small hardening (softening) and one that is near the minimum of the $T=0$ curve will show a very small hardening first and then a big softening. In every case the shift of the phonon line will mainly take place in the region $[T_c, \frac{2}{3}T_c]$.

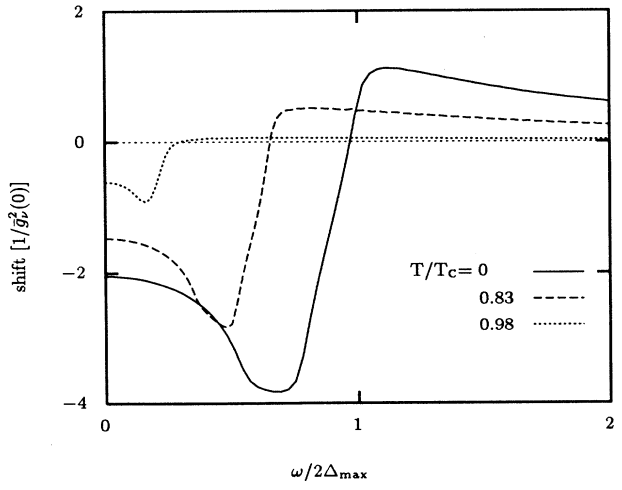

FIG. 3. Real part of $\delta\omega_{v0}$ for the s-wave anisotropy for different temperatures for $V_0=0$, $V_1=-0.229$ (in eV) and $\mu'\simeq-2.22$.

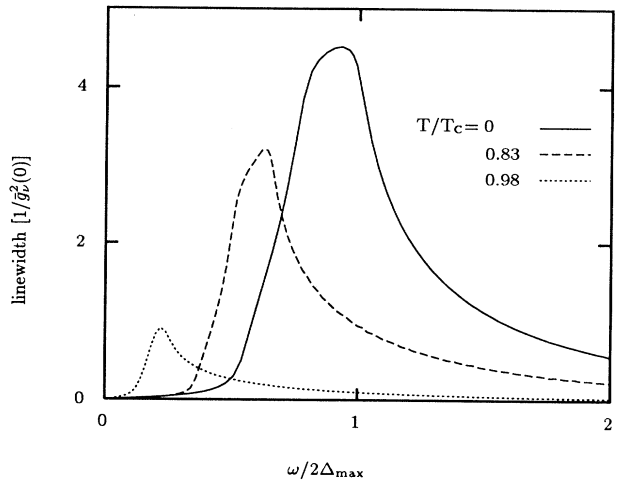

FIG. 4. Imaginary part of $\delta\omega_{v0}$ for the s-wave anisotropy for different temperatures $V_0=0$, $V_1=-0.299$ (in eV) and $\mu'\simeq-2.22$.

B. d-wave anisotropy

Figures 5 and 6 show the phonon shift and linewidth, respectively, for a pure d-wave anisotropy of the gap as a function of temperature. In the model considered we could not find values of the parameters V_0 and V_1 that give $\Delta_0\neq0$ and $\Delta_x=-\Delta_y\neq0$ at the same time. This case was, however, treated in Ref. 28 for a modified model, and the conclusions do not change from those presented here. The essential characteristic feature of the phonon shift for the d-wave case is that the singularity near the maximum of the gap is completely washed out by the anisotropy. This behavior is not altered for finite temperatures. Consequently, the value of the maximal phonon shift is strongly reduced in this case. The linewidth of

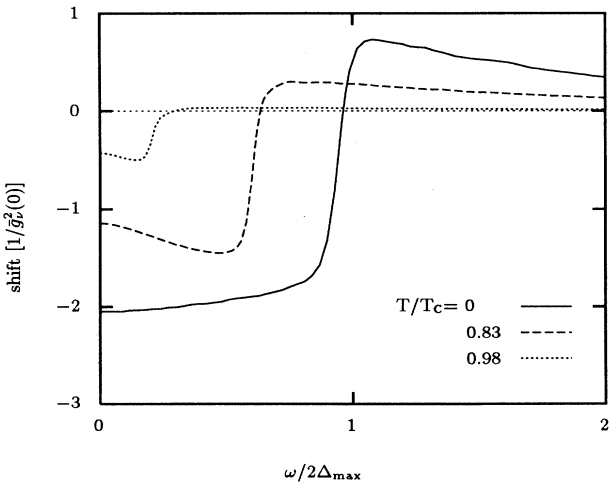

FIG. 5. Real part of $\delta\omega_{v0}$ for different temperatures for $V_0=0$, $V_1=-0.299$ (in eV) and $\mu'=-1.35$.

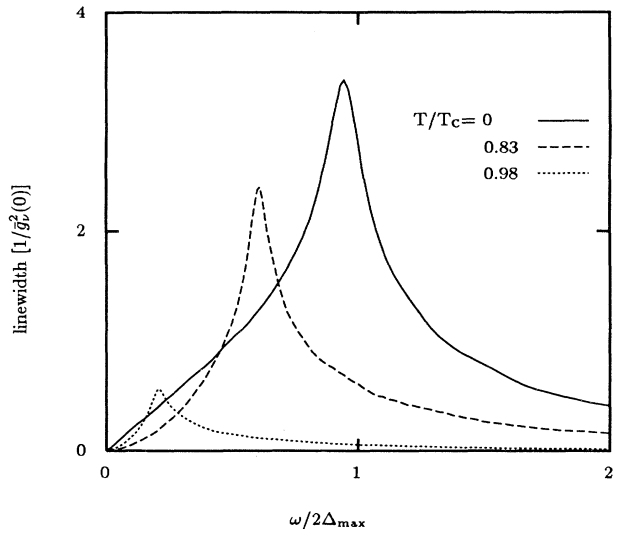

FIG. 6. Imaginary part of $\delta\omega_{\nu 0}$ for different temperatures $V_0=0$, $V_1=-0.299$ (in eV) and $\mu'=-1.35$.

the phonon for the d-wave anisotropy of the gap is also quite different from the s-wave case. Comparing Figs. 1 and 5, one notes that for a d-wave anisotropy the broadening of the linewidth of low-energy phonons is finite. For $T=0$ the increase with energy is nearly linear. This contrasts to the results found in the framework of BCS or Eliashberg theory for an isotropic gap as well as for an anisotropic s-wave gap. There the linewidth is zero below a critical value of the energy (2Δ for the BCS case) as already mentioned. A last property of the d-wave anisotropy is that in contrast to the phonon shift resulting from an s-wave anisotropy the curve in Fig. 5 shows a sharp transition from a softening to a hardening at $\Delta_{\max}$. This behavior is similar to the strong-coupling calculation[17] for $T=0$. At higher temperatures, however, the transition becomes smooth in strong coupling, while in the d-wave case it is still sharp. We have also performed calculations for the mixed state $\Delta_0=0$, $\Delta_x\neq\pm\Delta_y\neq 0$. The phonon shift and broadening have essentially the same features as the d-wave case (in particular, the absence of the minima in $\Delta\omega$ and the linear increase of $\Delta\gamma$ for small energies at $T=0$).

C. Influence of interplanar pairing

Until now we have calculated the renormalization of the $\mathbf{q}=0$ phonons below T_C for an anisotropic two-dimensional superconducting order parameter. We have thus only considered the gap anisotropy resulting from the intraplanar coupling and neglected the influence of the interplanar anisotropic pairing. The effect of the (ab,c) anisotropy on different properties of high-T_c superconductors was studied by many groups (see, e.g., Refs. 29 and 30). For the renormalization of the phonon energy, the influence of the k_z-dependent gap was studied in Ref. 18, assuming isotropy in the plane. Here we would like to study the effect, considering, however, the in-plane anisotropy of the gap as well. For this we added an interplanar interaction of the form $V_z\cos(k_z)$ to (34). The solutions of the gap equation for small V_z have then the same dependence on k_x,k_y as in the previous section, but with an additional part of the form $\Delta_z\cos(k_z)$. The solutions of the gap equation are given in Table I. We restricted the study of the interplanar interaction to realistic values of the ratio Δ_z/Δ_x ($\lesssim 0.1$). The renormalization is shown in Figs. 7 and 8. No solutions were found with $\Delta_z\neq 0$ and d-wave symmetry for the in-plane part of the gap. We compare the pure s-wave anisotropic case (dotted curve; this curve is the same as the dotted curve of Figs. 1 and 2) with the situation were a k_z component is added to the isotropic (dashed line) and the in-plane anisotropic (solid line) gap. The main difference for the shift (Fig. 7) is that the transition from softening to hardening is slightly sharper when $\Delta_z\neq 0$. For the isotropic case the value of the maximal softening is reduced, whereas for the in-plane anisotropic case it is slightly enlarged. Concerning the imaginary part, one notes that the k_z component of the gap gives a sharper maxima and that the value of the maximal broadening shows the same features than the value of the maximal softening. However, as one can see from the curves, the effect of the c anisotropy is negligible for realistic values of the parameters. The influence of different symmetries of the gap on the renormalization of the phonon energy can thus be studied, neglecting the interplanar pairing interaction.

IV. DISCUSSION

From all the results presented in the last section, one can draw some conclusions on the strength of the electron-phonon interaction constant and on the type of anisotropy the gap must (not) have to explain the experi-

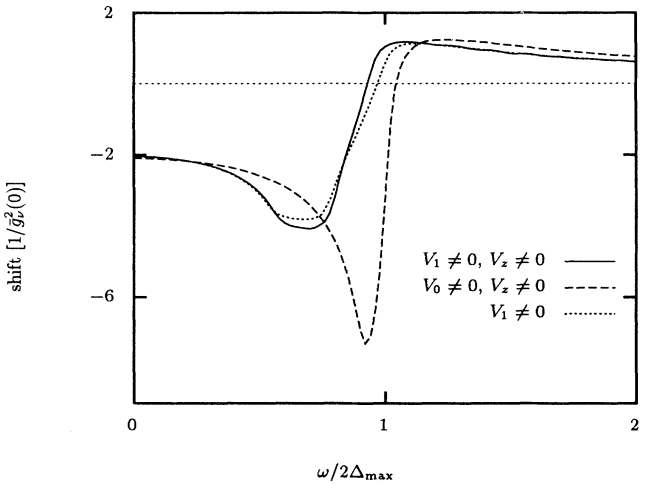

FIG. 7. Real part of $\delta\omega_{\nu 0}$ taking into account interplanar coupling. $V_0=0$, $V_1=-0.29$, $V_x=-0.007$ (solid line); $V_0=-0.247$, $V_1=0$, $V_z=-0.009$ (dashed line); $V_0=0$, $V_1=-0.299$, $V_z=0$ (dotted line) (in eV). Parameters are such that $\Delta_z/\Delta_x\simeq 0.1$. $\mu'=-2.22$, $T=0$.

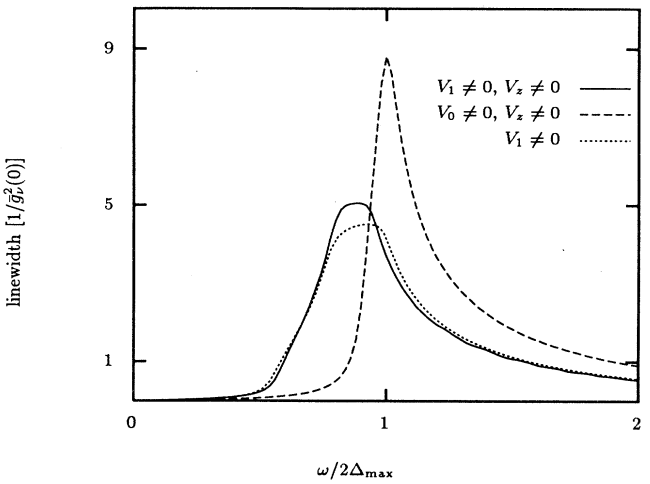

FIG. 8. Imaginary part of $\delta\omega_{\nu 0}$ taking into account interplanar coupling. Same parameters as for Fig. 7.

mental renormalization of the Raman- and IR-active phonon lines. We first analyze the pure *d*-wave anisotropy shown in Figs. 5 and 6. As one can see, both curves are rather inconsistent with the experiments done on $R\mathrm{Ba_2Cu_3O_{7-\delta}}$ (R = rare earth). There are no more minima appearing in the shift of the phonon energy, and thus all the phonons below the maximum of the gap should show the same small softening, which is not observed. More important, however, is that the linewidth of the phonons is gradually increasing from zero to its maximal value, whereas it was experimentally shown that for low temperatures the phonons with small energy experience only a negligible change of the linewidth.[31] It thus seems that neither a *pure d*-wave anisotropy nor a gap which has an isotropic part added to the *d*-wave component[20] can account for the anomalous renormalization of the Raman- and IR-active phonons in $\mathrm{YBa_2Cu_3O_{7-\delta}}$. The same conclusion holds for the mixed state of the gap. In contrast to these symmetries, an *s*-wave anisotropic gap with $\Delta_0=0$ does not have the above-mentioned inconvenience. It was already shown[17] that the weak-coupling calculation done with an isotropic (*s*-wave) gap does not fit the experimental curves. We thus have to consider the possibility of an *s*-wave anisotropy. As one can see in Fig. 2, there is always a minimal value of the energy below which the superconductivity-induced broadening of the linewidth vanishes. The real part (Fig. 1) of the renormalization has a minima too, which is, however, smaller than for the pure isotropic case, but still gives the order of magnitude of the measured shifts. We notice here the fact that we do not need to assume scattering to impurities[17] to obtain the right magnitude of $\Delta\omega_{\nu 0}$ and $\Delta\gamma_{\nu 0}$. The electron-phonon coupling also does not need to be strong. The presence of anisotropy reduces in a natural way this renormalization and reproduces the qualitative features of the experiments as was suggested in Ref. 32 by supposing a mode-dependent gap (one for each phonon mode) present in the system. Looking at the curves shown in Figs. 1 and 2 more carefully, one can further conclude that a pure *s*-wave anisotropic gap ($\Delta_0=0$) does not give the best fit to the measurements because the transition from a softening to a hardening as well as the transition from zero to the maximal broadening of the linewidth are too smooth. It thus suggests that a better fit to the renormalization of the Raman- and IR-active phonon modes can be given by a gap function that has a symmetry between the pure isotropic ($\Delta_0\neq 0$, $\Delta_x=\Delta_y=0$) and the pure anisotropic ($\Delta_0=0$, $\Delta_x=\Delta_y\neq 0$) *s*-wave cases. Indeed, the dashed curve in Figs. 1 and 2 shows in this intermediate case a relative sharp transition from softening to hardening, a threshold for the existence of a finite linewidth broadening, a pronounced minima for the superconductivity induced shift, and a pronounced maxima in the broadening of the linewidth. At this point one can also mention that according to our calculations the experimentally determined value of the gap in Ref. 31 corresponds to the maximum of the anisotropic gap function. Taking into account all these facts and although the model used for the numerical part of the calculations is obviously too rough to be fully quantitative, one can estimate the coupling constant $g_\nu(\mathbf{q}=0)$ from the fit of the experimental frequency shifts or linewidths.[31] The order of magnitude obtained is $|g_\nu(\mathbf{q}=0)|=0.01$ eV. Taking into account that the total number of optical phonons is large (about 10), one can conclude that the total electron-phonon coupling strength is moderate (about 0.1 eV).

The experiments measuring the order parameter have not been sensitive enough up to now to establish if the anisotropy of the gap extends over the whole Brillouin zone or if the $\mathbf{k}$ dependence is limited to a relatively small region and is otherwise constant. In our model the gap $\Delta_{\mathbf{k}}=\Delta_0+\Delta_x\cos(k_x)+\Delta_y\cos(k_y)$ is a smooth function. As soon as the anisotropic part appears when the parameters of the pairing potential are changed, the whole Brillouin zone is affected by the anisotropy. The results of our calculations show that it is this anisotropic part that damps the minima and maxima of $\Delta\omega$ and $\Delta\gamma$, respectively, through the destruction of the singularity at the upper edge of the electronic density of states. On the other hand, they suggest that the $\mathbf{k}$ dependence of the gap should be limited to a smaller region of the Brillouin zone than in the present model so as to ensure a sharp enough transition from a vanishing to a maximal linewidth renormalization as well as from a softening to a hardening of the phonon lines to fit the experimental curves at best. However, the region of the Brillouin zone in which the gap is nonconstant cannot be too small. Indeed, if this were the case, then the energy at which the transitions (e.g., from softening to hardening) occur would no longer be located at $2\Delta_{max}$, but at the energy of the flat dominant part of the gap, which must not be greater than about 5 meV as shown in experiments. In this last case the 340-$\mathrm{cm^{-1}}$ mode, for example, would experience a hardening below T_c, which contradicts the experiments.

One possibility to obtain a gap function that has all the above properties is to consider long-range Coulomb in-

teractions.[10] Another example was given in Ref. 9. All the presented conclusions are naturally only valid if the electron-phonon matrix element depends solely on the phonon wave vector **q** and if one restricts the possible symmetries of the order parameter to either the s-wave, d-wave, or mixed case. Solutions of the gap equation, for example, of the type $s+id$ (Refs. 33 and 34) were not considered.

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