Tunneling inversion with an excitonic contribution

F. Marsiglio* and J. P. Carbotte
Physics Department, McMaster University, Hamilton, Ontario, Canada L8S4M1
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We calculate the quasiparticle density of states in a phonon plus higher-energy exciton model. Without explicitly including the excitons in the process, the data are inverted to recover an effective phonon spectral density which is found to be very nearly the input distribution divided by $(1+\lambda_{ex})$ where λ_{ex} is the exciton contribution to the mass renormalization. A negative effective Coulomb "repulsion" is also obtained and the effective microscopic parameters do not reproduce exactly the initial density of states. Finally, the size of the structure in the region of the effective distribution is found to be enhanced by the presence of the exciton peak.

Phonon structure as large in size as that in Pb has been observed in tunnel junctions of $Ba(Pb,Bi)O_3$ which has a critical temperature around 12.0 K. An attempt to invert the data so as to recover microscopic parameters failed.[1] No details are given of this failure. Presumably, a negative effective Coulomb repulsion parameter μ^* resulted and the effective parameters did not reproduce well the initial data.

There is as yet no consensus as to the mechanism that is responsible for the superconductivity of the high-T_c oxides.[2] One possibility that is being explored is that it is a combined phonon plus excitonic mechanism.[3-6] In this picture, La-Sr-Cu-O would have a significant phonon contribution and an attendant isotope effect as is measured, while Y-Ba-Cu-O would be mainly excitonic with no isotope effect. In this work, we wish to consider a combined phonon and exciton model and study the quasiparticle density of states in this case. We also wish to invert the data assuming a pure phonon system so as to understand what the signature of the exciton peak might be in such a procedure.

To calculate the density of quasiparticle states normalized to the single-spin electronic density of states at the Fermi energy $[N(0)]$,

$$\frac{N(\omega)}{N(0)}=\mathrm{Re}\left(\frac{\omega}{\sqrt{\omega^2-\Delta^2(\omega)}}\right), \tag{1}$$

we need the complex frequency-dependent gap $\Delta(\omega)$ which follows from the Eliashberg equations on the real frequency axis at zero temperature[7]

$$\Delta(\omega)Z(\omega)=\int_0^\infty d\omega'\left[\mathrm{Re}\left(\frac{\Delta(\omega')}{\sqrt{\omega'^2-\Delta^2(\omega')}}\right)\right][K_+(\omega,\omega')-\mu^*\theta(\omega_c-\omega')] \tag{2}$$

and

$$\omega[1-Z(\omega)]=\int_0^\infty d\omega'\left[\mathrm{Re}\left(\frac{\omega'}{\sqrt{\omega'^2-\Delta^2(\omega')}}\right)\right]K_-(\omega,\omega'), \tag{3}$$

with

$$K_\pm(\omega,\omega')=\int_0^\infty d\Omega\, g(\Omega)\left(\frac{1}{\omega'+\omega+\Omega+i0^+}\pm\frac{1}{\omega'-\omega+\Omega+i0^+}\right), \tag{4}$$

where $g(\Omega)$ is the sum of an electron-phonon spectral density denoted by $\alpha^2F(\Omega)$ and an exciton contribution $P(\Omega)$ presumably at higher frequencies. Given $g(\Omega)$ and the Coulomb pseudopotential μ^* with a fixed cutoff (ω_c) we can calculate the quasiparticle density of states $N(\omega)$—a quantity that is measured in tunneling experiments. Conversely, given $N(\omega)$ we can recover, through an inversion procedure, the kernel $g(\Omega)$ and μ^* following Galkin, D'yachenko and Svistunov[8] and Mitrovic and Carbotte.[9,10]

In Fig. 1, we show our input spectrum for $g(\Omega)$. The lower-frequency distribution is the tunneling-derived electron-phonon spectral density for pure Pb (Ref. 7) reduced by a factor of 0.83 so that its mass-renormalization value is $\lambda_{e\text{-ph}}=1.28$. The high-frequency Lorentzian peak is meant to simulate a excitonic contribution and has a mass enhancement factor of $\lambda_{ex}=0.67$. For these parameters the zero-temperature gap edge $\Delta_0\cong 7.3$ meV. The quasiparticle density of states that is obtained in this way is shown in Fig. 2 (solid curve) in the low-energy region. If the data in this region are inverted without reference to the excitonic structure which appears at high energy we recover very nearly the input electron-phonon spectral density $\alpha^2F(\Omega)$ divided by the renormalization factor

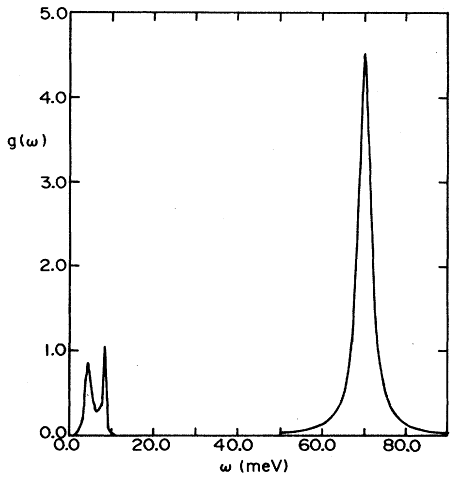

FIG. 1. The Eliashberg spectral density $g(\omega)$ used in this work. It is made up of the sum of an electron-phonon contribution $\alpha^2F(\omega)$ at low energy and an excitonic part $P(\omega)$ at higher energy centered around 70 meV (Lorentzian peak).

$(1+\lambda_{ex})$. This was expected from some previous work.[11,12] The first signature of the effect of the exciton peak is that this effective phonon spectral density

$$\alpha^2_{\rm eff}F(\Omega)\cong\frac{\alpha^2F(\Omega)}{1+\lambda_{ex}} \tag{5}$$

is very small for a gap edge (Δ_0) value of ~ 7.3 meV. Secondly, a negative effective Coulomb pseudopotential $\mu^*_{\rm eff}(-0.176)$ is required to reproduce this value of Δ_0. This negative value of $\mu^*_{\rm eff}$, of course, simulates the presence of the excitonic peak at higher energies which is not used in the inversion. The third important signature is that the effective kernels cannot reproduce exactly the original quasiparticle density of states as is shown in the dashed curve of Fig. 2. While it overlaps the solid curve, there are some differences, and we must conclude that no effective phonon kernel plus negative μ^* can ever reproduce exactly the effect of a phonon plus exciton kernel. We would, therefore, take the failure of the inversion procedure, as outlined here, as indirect evidence for an additional high-energy mechanism adding on to a phonon contribution. This second mechanism need not be excitonic in origin. It need only occur at higher energies and be describable, in a first approximation, by some high-energy peak in the Eliashberg equations.

The effective electron-phonon mass renormalization corresponding to the spectral density (5) is small and approximately 0.77. On its own, it would give a small gap edge and a small amount of phonon structure. On the other hand, the original phonon kernel plus exciton leads to a large gap Δ_0 and considerable structure in the phonon region. That this is the case can be seen by comparing Figs. 3 and 4.

In Fig. 3, we show results of several runs using, in all cases, a Pb spectrum with $\mu^*\cong 0.08$. Only the phonon re-

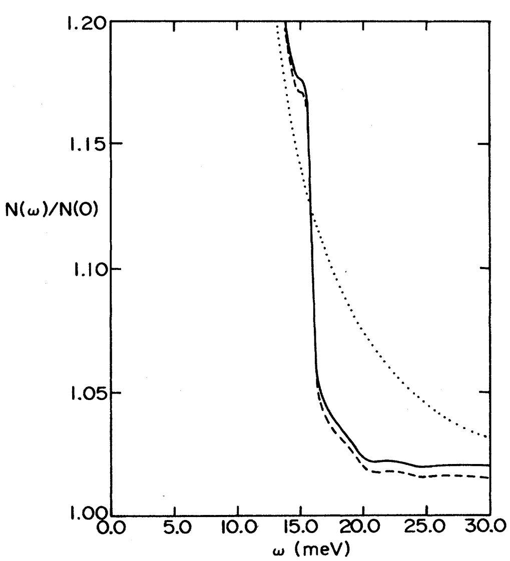

FIG. 2. The quasiparticle density of states (solid curve) obtained from the combined phonon and exciton spectrum of Fig. 1. For $\mu^*=0.1$, we get a gap edge of 7.27 meV. Superimposed on the same figure are results (dashed line) obtained from the effective Eliashberg kernels ($\lambda^{\rm eff}_{eph}\cong 0.77$ and $\mu^*_{\rm eff}\cong -0.176$) derived by inversion of the solid curve. The effective kernels do not reproduce the density of states exactly. The dotted curve is the BCS density of states given by Eq. (6) and is included for reference.

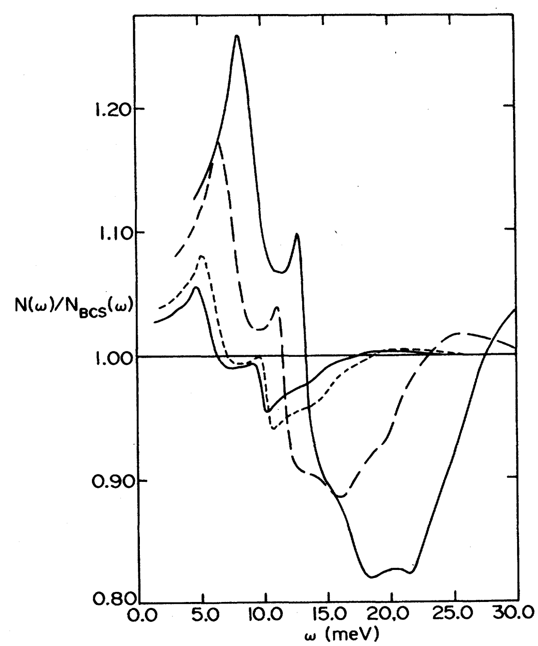

FIG. 3. The ratio of the quasiparticle density of states $N(\omega)$ to its BCS value $N_{\rm BCS}(\omega)$ for various systems. In all cases $\mu^*\cong 0.08$ and the Pb electron phonon spectral density is used but with a multiplicative factor of B included so as to increase or decrease the coupling. The curves exhibit more structure as B increases with $B=0.83$, 1.0, 3.02, and 4.57 and the gap edge Δ_0 is, respectively, 1.25, 1.63, 3.02, and 4.57 meV.

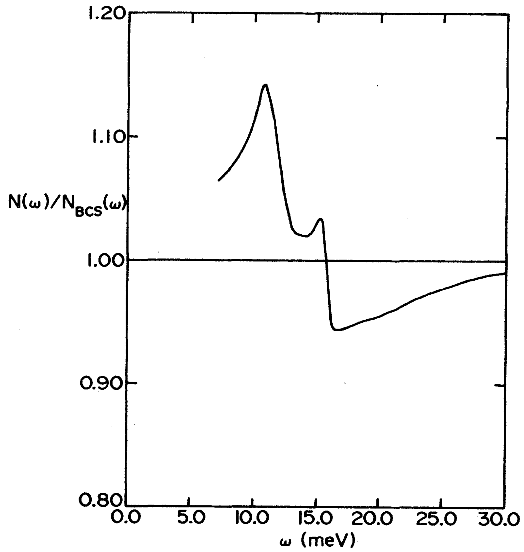

FIG. 4. The ratio of the quasiparticle density of states $N(\omega)$ to its BCS value $N_{BCS}(\omega)$ for the combined phonon plus exciton spectrum of Fig. 1. This case corresponds to $B=0.83$ and has a gap edge of $\Delta_0=7.27$ meV. Note that the amount of structure obtained is much larger than for the corresponding $B=0.83$ case of Fig. 3.

gion is shown and what is plotted is $N(\omega)$ divided by the Bardeen-Cooper-Schrieffer (BCS) density of states

$$\frac{N_{BCS}(\omega)}{N(0)}=\mathrm{Re}\left[\frac{\omega}{\sqrt{\omega^2-\Delta_0^2}}\right], \tag{6}$$

which involves only the gap edge. The various curves shown start at their respective gap edges Δ_0 and are for $B=0.83$, $B=1$, $B=2.83$, and $B=3.83$ in order of increasing size. Here, B is a factor multiplying the original Pb $\alpha^2F(\Omega)$ so as to increase or decrease its value. The gap edges are, respectively, 1.25, 1.63, 3.02, and 4.57 meV and correspond to ever increasing electron phonon spectral density. These curves are to be compared with the curve in Fig. 4 which applies to the case of phonon plus exciton which we have previously described. It has a $\Delta_0=7.27$ meV for a $\mu^*=0.1$. It is clear that the amount of structure obtained in the phonon region is much larger than obtained for the same $\alpha^2F(\Omega)$ alone (i.e., without an additional exciton peak) and very much larger than for $\alpha^2_{\mathrm{eff}}F(\Omega)$. It is only slightly smaller than the $B=2.83$ case. As first pointed out by Kus and Carbotte[13] within the context of hydrogen in aluminum, a high-energy peak in the Eliashberg kernel, which goes unrecognized in a tunneling experiment, effectively enhances the structure in the phonon region at lower energy and could lead one to think that the phonon kernel is larger than it actually is.

In conclusion, inversion of tunneling data for a system with an unrecognized high-energy contribution to the Eliashberg kernels leads to an effective electron-phonon spectral density which is reduced by a factor of $(1+\lambda_{ex})$ and a negative effective Coulomb repulsion parameter. This last parameter incorporates some of the effect of the second higher-energy attractive mechanism for Cooper pair formation. These effective microscopic parameters can never, however, reproduce perfectly the initial quasiparticle density of states from which they are derived. Finally, the amount of structure found in the phonon region is, in a very specific sense, enhanced over the amount that would be present from the phonon kernel alone with the higher-energy part left out and could lead one to believe, if the higher-energy structure is not recognized, that the phonon spectral density is larger than it actually is.

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*Present address: University of California at San Diego, La Jolla, CA 92093.

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