Boson structure in the quasiparticle density of states of superconductors with nodes in the gap

C. Jiang and J. P. Carbotte
Physics Department, McMaster University, Hamilton, Ontario, Canada L8S 4M1

R. C. Dynes
Physics Department 0319, University of California at San Diego, La Jolla, California 92093
(Received 31 August 1992; revised manuscript received 30 November 1992)

Within a generalized Eliashberg formalism, valid for exotic pairing states of a *D*-wave superconductor, we have studied how details of the electron-boson spectral density responsible for superconductivity manifest themselves as structure in the quasiparticle density of states. We find that the boson structure, which is to be measured relative to the energy defined by the peak in this function, shifts very little when resonant impurity scattering is introduced. Impurity scattering, however, can fill in the density of states at zero frequency and in the region below the peak which defines a gap value. Finite-temperature effects further smear this low-frequency region, as is expected from the well-studied isotropic case. Some comments on comparison with experiments are also given.

I. INTRODUCTION

In *S*-wave isotropic conventional superconductors, the current (I) voltage (V) characteristics of a tunneling junction can be used to measure the quasiparticle density of states as a function of energy ω. At low temperatures, this function shows a sharp onset at a definite gap (Δ) value, which is followed by a square root type singularity and boson structure at higher energies.[1-3] This structure corresponds to the detailed shape of the electron-boson spectral density $\alpha^2F(\omega)$ responsible for the superconductivity, and the phonon spectral density in conventional superconductors can be recovered from inversion of tunnelling data.[1] In the high-T_c oxides, even in the reproducible data of Valles *et al.* on $YBa_2Cu_3O_7$,[4] a large zero bias anomaly is observed with considerable associated smearing in the gap region and strong attenuation of the expected peak at the gap position if interpreted in an *S*-wave model. At higher energies, some bosonlike structure is observed. The precise origin of the smearing in the gap region and of the bosonlike structure is not yet known and it could have several possible explanations.[4]

Recently, several authors have again put forward arguments in favor of *D*-wave superconductivity in the copper oxides stabilized through antiferromagnetic spin fluctuations in the Cu-O planes.[5-16] In such theories, the gap region is filled in naturally although, at zero frequency, a zero value for the quasiparticle density of states is still predicted. On the other hand, it is known from much work on resonant impurity scattering in *p*-wave superconductors that the quasiparticle density of states at $\omega=0$ becomes finite in the unitary scattering limit[17-26] of normal impurity scattering.

In this paper, we wish to consider *D*-wave-like superconductivity within an Eliashberg formalism so as to study several effects, not present in the BCS approaches that have been used so far. First, we will be interested in how boson structure gets reflected in the quasiparticle density of states in a model superconductor which exhibits zeros in the gap as a function of momentum on the Fermi surface. We also want to know how boson structure is changed when impurity scattering is introduced so as to fill in the density of states at $\omega=0$. In the course of this investigation, we are led to consider a density of states which has many of the features measured in present tunnelling data for $YBa_2Cu_3O_7$ tunnelling. Such data is certainly not inconsistent with *D*-wave-like pairing with the stabilizing bosons presumably the antiferromagnetic paramagnons or spin fluctuations although results are quite independent of such an assumption. Finally, we study how finite-temperature effects further smear the gap region due to depairing.

II. FORMALISM

The pairing energy $\tilde{\Delta}_{\mathbf{p}}(\omega)$ for an electron of momentum $\mathbf{p}$ on the Fermi surface, as a function of real frequency (ω) and the renormalization $\tilde{\omega}_{\mathbf{p}}(\omega)$ (including impurity scattering in a multiple scattering T-matrix approximation) are[27-31]

$$\tilde{\Delta}_{\mathbf{p}}(\omega)=\pi T\sum_{m=0}^{\infty}\left\langle[\lambda_{\mathbf{pp}'}(\omega-i\omega_m)+\lambda_{\mathbf{pp}'}(\omega+i\omega_m)]\frac{\tilde{\Delta}_{\mathbf{p}'}(i\omega_m)}{\sqrt{\tilde{\omega}^2_{\mathbf{p}'}(i\omega_m)+\tilde{\Delta}^2_{\mathbf{p}'}(i\omega_m)}}\right\rangle'$$
$$+i\pi\int_{-\infty}^{\infty}dz\left\langle\alpha^2F_{\mathbf{pp}'}(z)[n(z)+f(z-\omega)]\frac{\tilde{\Delta}_{\mathbf{p}'}(\omega-z)}{\sqrt{\tilde{\omega}^2_{\mathbf{p}'}(\omega-z)-\tilde{\Delta}^2_{\mathbf{p}'}(\omega-z)}}\right\rangle'+i\pi\Gamma\frac{D(\omega)}{C_0^2+D^2(\omega)+\Omega^2(\omega)} \quad (1)$$

and

$$\tilde{\omega}_{\mathbf{p}}(\omega)=\omega+\pi T\sum_{m=0}^{\infty}\left\langle[\lambda_{\mathbf{pp}'}(\omega-i\omega_m)-\lambda_{\mathbf{pp}'}(\omega+i\omega_m)]\frac{\tilde{\omega}_{\mathbf{p}'}(i\omega_m)}{\sqrt{\tilde{\omega}^2_{\mathbf{p}'}(i\omega_m)+\tilde{\Delta}^2_{\mathbf{p}'}(i\omega_m)}}\right\rangle'$$
$$+i\pi\int_{-\infty}^{\infty}dz\left\langle\alpha^2F_{\mathbf{pp}'}(z)[n(z)+f(z-\omega)]\frac{\tilde{\omega}_{\mathbf{p}'}(\omega-z)}{\sqrt{\tilde{\omega}^2_{\mathbf{p}'}(\omega-z)-\tilde{\Delta}^2_{\mathbf{p}'}(\omega-z)}}\right\rangle'+i\pi\Gamma\frac{\Omega(\omega)}{C_0^2+D^2(\omega)+\Omega^2(\omega)} \tag{2}$$

with

$$\lambda_{\mathbf{pp}'}(\omega)=-\int_{-\infty}^{\infty}\frac{\alpha^2F_{\mathbf{pp}'}(\Omega)d\Omega}{\omega-\Omega+i0^+}\ , \tag{3}$$

$$D(\omega)=\left\langle\frac{\tilde{\Delta}_{\mathbf{p}'}(\omega)}{\sqrt{\tilde{\omega}^2_{\mathbf{p}'}(\omega)-\tilde{\Delta}^2_{\mathbf{p}'}(\omega)}}\right\rangle'\ , \tag{4a}$$

and

$$\Omega(\omega)=\left\langle\frac{\tilde{\omega}_{\mathbf{p}'}(\omega)}{\sqrt{\tilde{\omega}^2_{\mathbf{p}'}(\omega)-\tilde{\Delta}^2_{\mathbf{p}'}(\omega)}}\right\rangle'\ , \tag{4b}$$

where $f(z)$ and $n(z)$ are the Fermi and boson thermal factors, respectively.

The band structure model used to derive these equations is one of free electrons in the x-y plane with effective mass m^* and a hopping probability t between planes which are stacked in the z direction. The electron dispersion relation is

$$\epsilon(\underline{k})=\frac{\hbar^2}{2m^*}(k_x^2+k_y^2)+t\cos(k_zc)\ , \tag{5a}$$

where c is the distance between planes in the z direction. For such a dispersion relation, the energy integrals in the gap equations can be carried out with the density of electron states assumed constant and pinned at its value at the Fermi energy $[N(0)]$. There is therefore nothing specific to the model (5a) in Eqs. (1) to (4) which apply to any case for which the electronic density of states is nearly constant in the energy range significant for superconductivity around the Fermi energy. In that sense, (5a) is introduced only to be more explicit. In the above equations, the angular brackets denote a Fermi surface average over angular parts and $\alpha^2F_{\mathbf{pp}'}(\omega)$ is the directional electron-boson spectral density for electron scattering from $\mathbf{p}$ to $\mathbf{p}'$ on the Fermi surface. It is this spectral density that mediates the pairing potential leading to superconductivity. Here it is modeled by an isotropic function of frequency $\alpha^2F(\omega)$ times an angular function of $\mathbf{p}$ and $\mathbf{p}'$. To get a superconducting gap parameter exhibiting nodes on the Fermi surface, the simplest model to take for this momentum dependence is

$$\alpha^2F_{\mathbf{pp}'}(\omega)=\cos(p_zc)\alpha^2F(\omega)\cos(p_z'c)\ , \tag{5b}$$

neglecting all other terms. The simple angular dependence assumed in (5b) for the pairing potentials is consistent with the isotropic dispersion curves in the x-y plane assumed in Eq. (5a). The precise origin of the spectral density (5b) does not concern us directly and our results do not depend sensitively on the choice of angular functions. What we are interested in here is the effect of this spectral density on the quasiparticle density of state when there are nodes in the gap as a function of direction on the Fermi surface. For specific consideration of the oxides, it would be more appropriate to consider a single Cu-O plane with a

$$[\cos(k_xa)-\cos(k_ya)]$$

dependence in the pairing potential. For this specific case, it has been shown by Nicol, Jiang, and Carbotte[32] that in a BCS theory such a model can be mapped exactly onto a $\alpha\cos(\theta)$ model with $\alpha=-(2-|\bar{\mu}|)$ for tight binding dispersion curves $\epsilon_k=-2t[\cos(k_xa)+\cos(k_ya)]-\mu$ with t the hopping integral and μ the chemical potential, all this provided the Fermi surface falls well away from the van Hove singularity in the electronic density of states. Also, $\bar{\mu}$ is dimensionless equal to $\mu/2t$.

The density of states in the superconducting state $N_S(\omega)$ normalized to its constant value in the normal state $N(0)$ is given by

$$\frac{N_S(\omega)}{N(0)}=\mathrm{Re}\left\{\left\langle\frac{\omega}{\sqrt{\omega^2-\Delta^2_{\mathbf{p}}(\omega)}}\right\rangle\right\}\ , \tag{6}$$

where $\Delta_{\mathbf{p}}(\omega)\equiv\omega\tilde{\Delta}_{\mathbf{p}}(\omega)/\tilde{\omega}_{\mathbf{p}}(\omega)$. The Eliashberg equations (1) and (2) contain a mixture of discrete Matsubara $(i\omega_n)$ and real frequencies (ω) with $i\omega_n=i\pi T(2n-1)$, $n=0,\pm1,\pm2,\ldots$ and T the temperature. To evaluate these equations explicitly so as to get the real frequency quantities $\tilde{\Delta}_{\mathbf{p}}(\omega)$ and $\tilde{\omega}_{\mathbf{p}}(\omega)$, we need to have as input the corresponding imaginary quantities $\tilde{\Delta}_{\mathbf{p}}(i\omega_n)$ and $\tilde{\omega}_{\mathbf{p}}(i\omega_n)$ which follow from the usual Eliashberg equation in Matsubara representation.[31]

$$\tilde{\Delta}_{\mathbf{p}}(i\omega_n)=\pi T\sum_{m-\infty}^{\infty}\left\langle\lambda_{\mathbf{pp}'}(i\omega_n-i\omega_m)\frac{\tilde{\Delta}_{\mathbf{p}'}(i\omega_m)}{\sqrt{\tilde{\omega}^2_{\mathbf{p}'}(i\omega_m)+\tilde{\Delta}^2_{\mathbf{p}'}(i\omega_m)}}\right\rangle'+\pi\Gamma\frac{D(n)}{C_0^2+[\Omega(n)]^2+[D(n)]^2} \tag{7}$$

and

$$\tilde{\omega}_{\mathbf{p}}(i\omega_n)=\omega_n+\pi T\sum_{m=-\infty}^{\infty}\left\langle\lambda_{\mathbf{pp}'}(i\omega_n-i\omega_m)\frac{\tilde{\omega}_{\mathbf{p}'}(i\omega_m)}{\sqrt{\tilde{\omega}^2_{\mathbf{p}'}(i\omega_m)+\tilde{\Delta}^2_{\mathbf{p}'}(i\omega_m)}}\right\rangle'+\pi\Gamma\frac{\Omega(n)}{C_0^2+[\Omega(n)]^2+[D(n)]^2} \tag{8}$$

with

$$\lambda_{pp'}(i\omega_n - i\omega_m) = \int_0^\infty \frac{2\omega\alpha^2 F_{pp'}(\omega)d\omega}{\omega^2 + (\omega_n - \omega_m)^2} , \tag{9}$$

$$D(n) = \left\langle \frac{\tilde{\Delta}_{p'}(n)}{\sqrt{\tilde{\omega}_{p'}^2(n) + \tilde{\Delta}_{p'}^2(n)}} \right\rangle' , \tag{10a}$$

and

$$\Omega(n) = \left\langle \frac{\tilde{\omega}_{p'}(n)}{\sqrt{\tilde{\omega}_{p'}^2(n) + \tilde{\Delta}_{p'}^2(n)}} \right\rangle' . \tag{10b}$$

The impurity parameters in the above equations are Γ and C_0. Γ measures the strength of the electron impurity scattering and is proportional to the impurity concentration while C_0 is related to the phase shift δ_0 by[14]

$$C_0 = \cot\delta_0 . \tag{11}$$

For $\delta_0 \to 0$, C_0 gets large and we recover the Born approximation while the other limit $C_0 = 0$ corresponds to $\delta_0 = \pi/2$ and is the unitary limit. In the numerical work that we present in the following section, we will use $C_0 = 0$ only because it gives the most significant filling in of the gap region in the quasiparticle density of states $N_S(\omega)/N(0)$, near $\omega \to 0$ for fixed Γ. We have, of course, done calculations for arbitrary values of C_0.

For our simple D-wave-like ansatz involving only the product $\cos(p_z c)\cos(p_z' c)$ for the **pp'** dependence of the spectral density $\alpha^2 F_{pp'}(\omega)$ on the Fermi surface, it is clear from Eq. (1) and (2) and from (7) and (8) that $\tilde{\Delta}$ and $\tilde{\omega}$ have the form

$$\tilde{\Delta}_p(\omega) = \tilde{\Delta}_0(\omega) + \tilde{\Delta}_1(\omega)\cos(p_z c) , \tag{12a}$$

$$\tilde{\omega}_p(\omega) = \tilde{\omega}_0(\omega) + \tilde{\omega}_1(\omega)\cos(p_z c) , \tag{12b}$$

$$\tilde{\Delta}_p(i\omega_n) = \tilde{\Delta}_0(n) + \tilde{\Delta}_1(n)\cos(p_z c) , \tag{12c}$$

$$\tilde{\omega}_p(i\omega_n) = \tilde{\omega}_0(n) + \tilde{\omega}_1(n)\cos(p_z c) . \tag{12d}$$

Thus Eqs. (1) and (2) reduce to four nonlinear coupled equations for $\tilde{\Delta}_0(\omega)$, $\tilde{\Delta}_1(\omega)$, $\tilde{\omega}_0(\omega)$, and $\tilde{\omega}_1(\omega)$ which require that we first solve the similar equations (7) and (8) for the four Matsubara quantities $\tilde{\Delta}_0(n)$, $\tilde{\Delta}_1(n)$, $\tilde{\omega}_0(n)$, and $\tilde{\omega}_1(n)$. Note that we have assumed that the spectral density (5b) contains a single anisotropic term with no corresponding isotropic contribution. For $T = T_c$, Eqs. (1) and (2) and Eqs. (7) and (8) become linearized in the gap and the first two terms in Eq. (1) and in (7), which involve the electron-boson spectral density directly, make no contributions to $\tilde{\Delta}_0$. It is only the impurities that contribute to this quantity. Our numerical work indicates that this is also true to a very good approximation for all temperature $T < T_c$. Also, since there is no isotropic term in our simple choice of $\alpha^2 F_{pp'}(\omega)$, at $T = T_c$ the two terms in Eqs. (2) and (8) involving the spectral density explicitly do not contribute to $\tilde{\omega}_0$. This would not be the case if an isotropic part had been added to Eq. (5b). Such model cases have been studied in the past.[13–16] A new parameter is, however, introduced into the theory, namely, the isotropic part of the spectral density $\alpha^2 F_{pp'}(\omega)$.

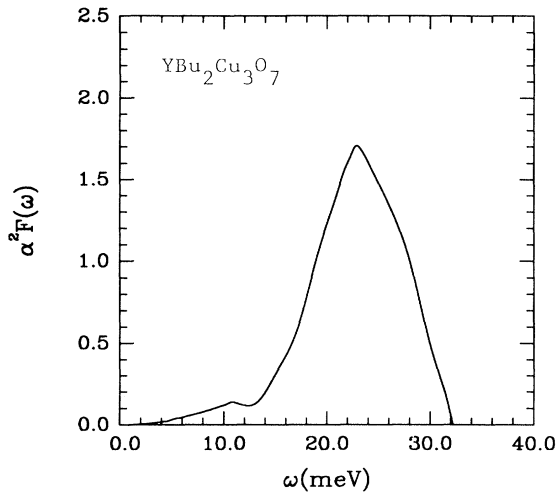

FIG. 1. Model electron-boson spectral density $\alpha^2 F(\omega)$ used in this work.

Due to our lack of information on this function, it is usually taken to be the same as the function $\alpha^2 F(\omega)$ used in the anisotropic part multiplied by some unknown scaling factor g. For simplicity, here we have left this term out entirely. To proceed with numerical work, we need to make a choice for the electron-boson spectral density $\alpha^2 F(\omega)$. In this paper, we use a scaling factor A times a function obtained by one of us (R.C.D.) from inversion of tunnelling data in $YBa_2Cu_3O_7$.[4] This inversion is based on conventional S-wave Eliashberg theory so that it is not at all clear what such a procedure might mean when no clear gap region is observed at small ω in which there are no states in the quasiparticle density of states. Nevertheless, since for definiteness we need to make some choice for $\alpha^2 F(\omega)$, we will use this data here, although the exact choice for $\alpha^2 F(\omega)$ is of little consequence to our main arguments and results except, in as much as, we wish to compare at the end with the data in $YBA_2Cu_3O_7$. The spectrum used peaks around 23 meV, is about 12 meV wide and ends at 32 meV and is shown in Fig. 1.

We can now present numerical results.

III. NUMERICAL RESULTS

As measured by the conventional strong coupling parameter T_c/ω_{ln}, the spectrum of Fig. 1 is in the extreme strong coupling regime with $T_c/\omega_{ln} \cong 0.4$. Here ω_{ln} is the usual Allen-Dynes[33] characteristic boson energy corresponding to our spectral density $\alpha^2 F(\omega)$. Because of this, we have experienced great difficulties in converging our real frequency programs, particularly when a finite amount of impurities is included. For this reason, we do not address first the specific case of $YBa_2Cu_3O_7$ but rather use the $\alpha^2 F(\omega)$ of Fig. 1 scaled so as to produce a critical temperature value of 50 K. The corresponding value for the strong coupling index T_c/ω_{ln} is now 0.21 which leads to satisfactory rapid convergence on the computers available to us. In Fig. 2, we show results for the resultant quasiparticle density of states $N_S(\omega)/N(0)$ as a func-

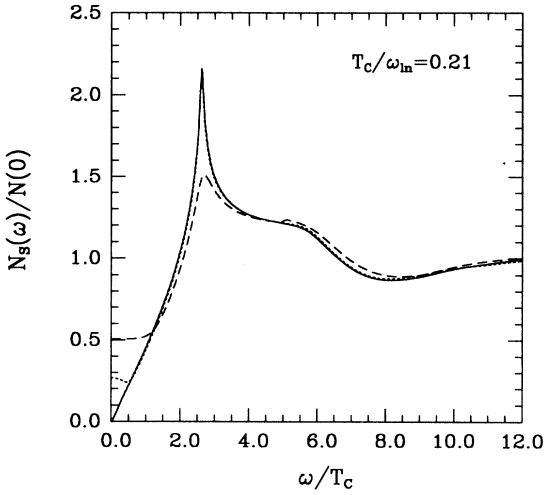

FIG. 2. The quasiparticle density of states $N_s(\omega)/N(0)$ as a function of normalized frequency ω/T_c for a D-wave-like superconductor for various impurity concentration in the unitary limit. The solid curve is for $\Gamma=0.0$ meV (pure limit), dotted curve for $\Gamma=0.10$ meV, and dashed for $\Gamma=0.50$ meV. $T_c=50$ K in all cases and the reduced temperature $T/T_c=0.1$ which is sufficiently low so as to be representative of a $T=0$ solution.

tion of ω/T_c. The solid curve applies to the pure case. The first thing to note is that the peak position, which we take as the gap position, falls approximately at $2\Delta/k_BT_c\cong 5.4$. This is close to the value observed in the experiment of Valles *et al.*[4] for $YBa_2Cu_3O_7$ although we should not be comparing directly because, in this case, $T_c=95$ K and not 50 K as in the results of Fig. 2. Note also that the minimum in the boson structure falls approximately at $\omega/T_c=8.0$ which is equal to the gap value as defined above by the peak in $N_s(\omega)/N(0)$, plus the value at which the maximum occurs in $\alpha^2F(\omega)$. This is perhaps surprising since, strictly speaking, there is no gap in the quasiparticle excitation spectrum for D wave. The rule for phonon structure, in this case, is, nevertheless, that it is to be measured from the position of the peak in $N_S(\omega)/N(0)$. It is clear from Fig. 2 (solid curve) that below the peak in $N_S(\omega)/N(0)$ there is substantial density of states although $N_S(\omega)/N(0)$ still goes to zero (almost linearly) as ω goes to zero. A prominent feature of the tunnelling data $YBa_2Cu_3O_7$, which cannot be explained with a D-wave gap in the pure limit, is the large zero bias anomaly at $\omega=0$. To get a finite value of $N_S(\omega)/N(0)$ at $\omega=0$, we need to include impurity scattering in the unitary scattering limit ($\delta_0=\pi/2$), i.e., $C_0=0$ in formulas (1) and (2) and (7) and (8) of the previous section. When impurities are included in this model, several features are to be noted in Fig. 2 dotted ($\Gamma=0.1$) and dashed ($\Gamma=0.5$) curves. The introduction of impurities does not significantly change the boson structure around $\omega/T_c\sim 8.0$. Secondly, the peak at $\omega/T_c\sim 2.5$ gets smeared and reduced as Γ increases but is not shifted significantly so that the ratio $2\Delta/k_BT_c$, defined by the position of this peak, remains almost the same for any Γ. Finally, the region near $\omega=0$ gets rapidly filled in with $N_S(\omega=0)/N(0)\cong 0.5$ in the case of $\Gamma=0.5$ meV. In summary, impurities attenuate somewhat the peak at the gap without changing much the phonon structure while, at the same time, filling in the region below the gap very significantly. Of course, the absolute value of T_c is also affected and reduced through the introduction of impurities. It should be noted in passing that in all the curves of Fig. 2, we have, in each run, readjusted the scaling on our $\alpha^2F(\omega)$ to get 50 K for all cases.

We now examine the effect of temperature on phonon structure and on the smearing of the gap region as T tends towards T_c. In Figs. 3(a) and 3(b), we show results for the quasiparticle density of states $N_S(\omega)/N(0)$ for different values of temperature. Figure 3(a) covers cases

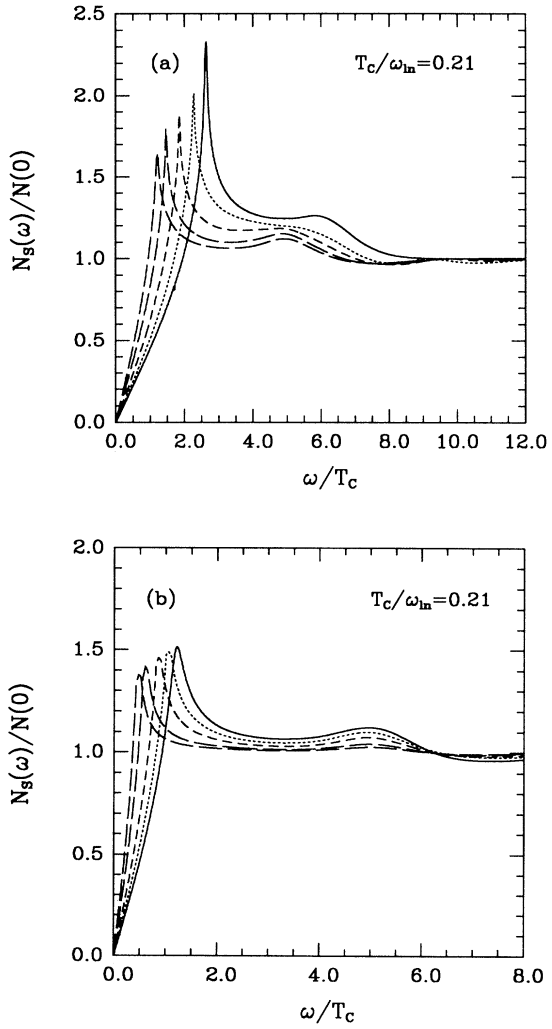

FIG. 3. The quasiparticle density of states $N_s(\omega)/N(0)$ as a function of normalized frequency ω/T_c for various reduced temperature T/T_c for a 50 K D-wave-like Eliashberg superconductor. In 3(a), $T/T_c=0.1$ (solid), 0.6 (dotted), 0.75 (short dashed), 0.85 (long dashed), and 0.9 (short dash-dotted). In 3(b), $T/T_c=0.9$ (solid), 0.925 (dotted), 0.95 (short dashed), 0.975 (long dashed), and 0.985 (second long dashed). All curves apply to the pure case.

from $T/T_c=0.1$ to 0.9 while Fig. 3(b) cover $T/T_c=0.9$ to 0.985, the region very near T_c. The curves of Fig. 3(a) are similar, in the gap region around the peak and below, to those shown by Pines[6] which he obtained in a BCS theory with planar D-wave anisotropy in the x-y plane instead of the layered z axis anisotropy considered here. In both theories, the peak position denoted by $\Delta_p(T)/\Delta_p(0)$ does not quite follow a BCS temperature variation. This is shown in Fig. 5 where the solid line is BCS temperature dependence and the open circles are our numerical results. These results fall substantially below the solid curve and the gap does not open up faster in our theory than in BCS. This is different from what is stated by Pines[6] about his work. Referring again to Fig. 3(a) the size of the peak (which remains sharp even for $T/T_c=0.9$) decreases with increasing temperature, an effect not seen in Pines[6] curves. Around $\omega=0$, however, our strong coupling results show little if any thermal smearing, an effect absent in BCS but expected in strong coupling. It was surprising to us that thermal smearing did not lead to a significant value of the density of state at $\omega=0$ even for $T/T_c=0.985$. Note that $T_c/\omega_{ln}=0.21$ in these curves. This is in the strong coupling regime and would lead to much more thermal smearing of the curves in the S-wave case. Of course, as T increases further, eventually $N_S(\omega)/N(0)$ at $\omega=0$ must go toward one. Finally, we note that as T increases towards T_c, the boson structure is attenuated as is the case for an S-wave isotropic superconductor.

If impurities are included in the unitary limit, $N_S(\omega=0)/N(0)$ will now be finite even for zero temperature. As the temperature is increased, we would expect this value to increase further and tend towards 1 as T goes towards T_c. In Fig. 4(a) and 4(b), we show results for $\Gamma=0.1$ and 0.5 meV, respectively, for a system with $T_c=50$ K and $T_c/\omega_{ln}=0.21$. As Γ is increased, it is clear that finite temperature effects at $\omega=0$ become progressively more significant but only slightly so. For $\Gamma=0.5$ meV, we see in Fig. 5 that the variation of the peak position with temperature follows more closely the BCS temperature variation of the gap than it did for the same case with $\Gamma=0.0$ (clean limit) and that the gap does, indeed, now open up faster than in BCS. The differences are, however, always small, and at lower temperatures, our results fall below the classic BCS temperature law. Even though our band structure model (5a) is too simple to apply directly to the case of $YBa_2Cu_3O_7$, and no attempt has been made to include explicitly the presence of chains, it is nevertheless interesting to choose parameters that might lead to behavior similar to what is observed in that case. This is done in our Fig. 6 which holds for a finite impurity concentration with $\Gamma=1.0$ meV.

We begin, however, with a discussion of the pure case $\Gamma=0$ in Eqs. (1) and (2), i.e., no impurity scattering. The first interesting feature of such a calculation with a gap of the form $\tilde{\Delta}_1(n)\cos(p_z c)$ is that the value of $\lambda=2\int_0^\infty[\alpha^2F(\omega)/\omega]d\omega$ needed to get a $T_c=95$ K is quite modest, namely, 1.7. This is in sharp contrast to the value of 5.1 needed to get the same T_c in an S-wave theory. We stress that if we had included an isotropic part to the spectral density in Eq. (5b) of the same order of magnitude as the anisotropic part (say, a number g times λ), we would have required a larger value of λ to obtain $T_c=93$ K in the D-wave-like case. This can be understood as follows: In a crude BCS-like approximation, the value of T_c is very roughly proportional to

$$T_c \sim e^{-1/\lambda}$$

for our d-wave model, while it would have been proportional to (again very roughly)

$$T_c \sim e^{-(1+\lambda g)/\lambda}$$

in the second case with an isotropic contribution of

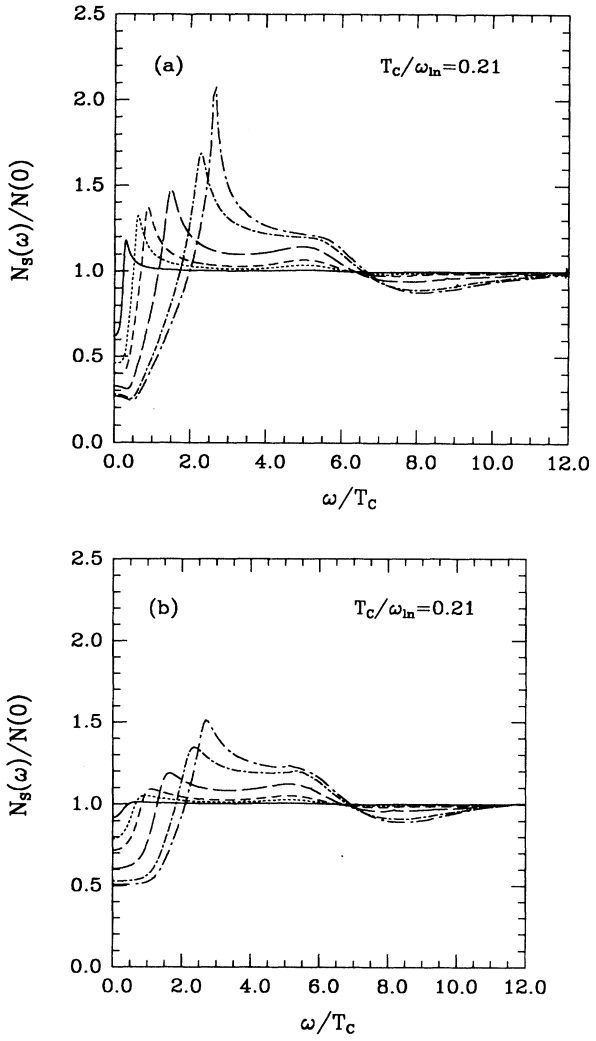

FIG. 4. The quasiparticle density of states $N_s(\omega)/N(0)$ as a function of normalized frequency ω/T_c for various values of reduced temperature T/T_c for a 50 K D-wave-like Eliashberg superconductor. The curves are for $T/T_c=0.1$ (long dashed dotted), 0.6 (short dashed dotted), 0.85 (long dashed), 0.95 (short dashed), 0.975 (dotted), and 0.995 (solid). Frame (a) is for $\Gamma=0.1$ meV in the T-matrix unitary limit for impurity scattering, while frame (b) is for $\Gamma=0.5$ meV. In both cases, $T_c/\omega_{ln}=0.21$ (fairly strong coupling case).

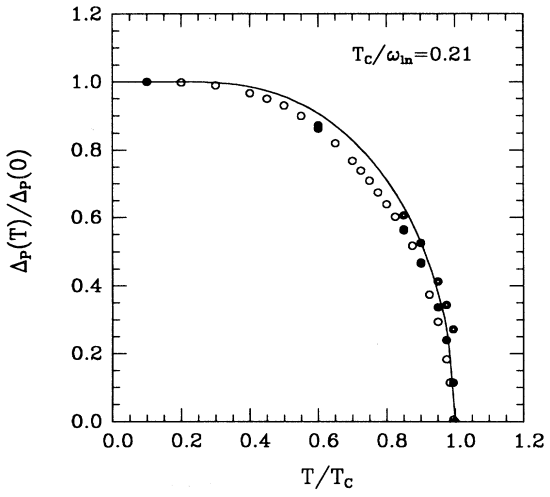

FIG. 5. The temperature variation of the position of the peak $\Delta_p(T)$ in the quasiparticle density of states. The solid curve for the dimensionless ratio $\Delta_p(T)/\Delta_p(0)$ vs reduced temperature T/T_c is the usual BCS temperature dependence of the gap. The open circles apply to our strong coupling case with $T_c=50$ K, $T_c/\omega_{ln}=0.21$, and $\Gamma=0.0$ (clean limit). The solid circles are for $\Gamma=0.1$ meV in the unitary T-matrix impurity scattering case while the heavy open circles are for $\Gamma=0.5$ meV.

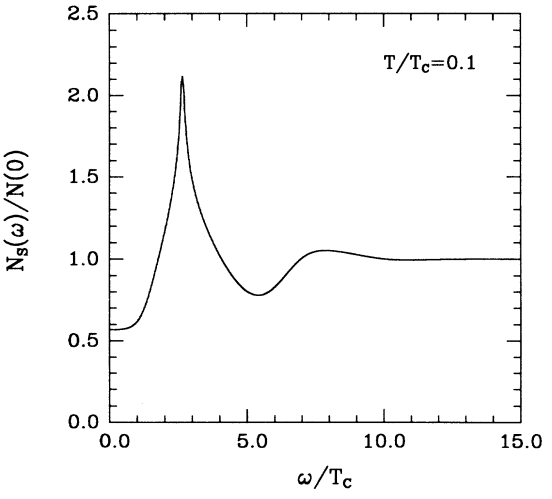

FIG. 6. The quasiparticle density of states $N_s(\omega)/N(0)$ as a function of normalized frequency ω/T_c for a D-wave like superconductor with $T_c=95$ K using the $\alpha^2F(\omega)$ of Fig. 1. The solid curve was not obtained from solutions of Eqs. (1) and (2) giving directly the gap as a function of real frequency. Instead, it was obtained from the Matsubara gaps upon solution of Eqs. (7) and (8) with Padé approximants to analytically continue to real frequencies. The impurity concentration needed to get a finite value of $N_s(\omega=0)/N(0)=0.57$ was $\Gamma=1.0$ meV. This reduces the intrinsic T_c value by about 30%.

strength g times λ included in (5b). For $g\neq 0$, a larger value of λ is required to achieve the same T_c value as for the $g=0$ case. We warn the reader, however, that the above agreement is not quantitative but does give some insight into why we require a λ equal to only 1.7 in the D-wave-like case as compared to 5.1 for S wave. Returning to Fig. 6, which applies to an impurity concentration $\Gamma=1.0$ meV, we see sharp boson structure in the quasiparticle density of states falling at about the boson energy in $\alpha^2F(\omega)$ plus the value of the position of the maximum in the curve which falls around 2.6 in units of ω/T_c. If the position of the peak is used to derive a value of the gap to T_c ratio $2\Delta/k_BT_c$, we get a value of approximately 5.2 for this ratio in agreement with experiment.[4] We stress that to obtain Fig. 6, we have not used Eqs. (1) and (2) because of convergence problems. Instead, we have worked in the Matsubara representation, i.e., used Eqs. (7) and (8) to obtain solutions for $\tilde{\Delta}_p(i\omega_n)$ and $\tilde{\omega}_p(i\omega_n)$ and then used Padé[34] approximants to analytically continue to real frequencies. This method is adequate for some applications but is not very good for phonon structure. This is not a great limitation here since we have already discussed boson structure in our previous figures where the real frequency axis solutions have been used. What we want here is a curve that can be compared fairly directly but only qualitatively with the data of Valles *et al.*[4] in $YBa_2Cu_3O_7$. To this end, we have used the $\alpha^2F(\omega)$ of Fig. 1 scaled so as to obtain a T_c of 95 K with an impurity content of $\Gamma=1.0$ meV. This impurity concentration reduces T_c by about 30% over its intrinsic pure value which would be well above 100 K in our model. On examination of Fig. 6, we can conclude that tunnelling characteristics quite similar to those observed in $YBa_2Cu_3O_7$, including the size and position of the boson structure, can be reproduced in a gap model with nodes on the Fermi surface due to the $\cos(k_zc)$ variation in the z direction, provided a small amount $\Gamma\sim 1.0$ meV of impurity scattering is included in the unitary scattering limit. Born impurity scattering does not fill in the gap region at all as effectively and so this case has not been explicitly discussed here. We stress that the exact form taken for the momentum variation of the gap over the Fermi surface is not in any way critical to our results. Models which include instead a D wave anisotropy in the copper oxide plane with tight binding bands for the x-y direction are expected to yield very similar results. Here we have used a $\cos(k_zc)$ form mainly for our convenience.

IV. CONCLUSIONS

Within Eliashberg theory for an anisotropic superconductor with nodes in the gap, we have studied how structure, due to the electron-boson spectral density, enters the quasiparticle density of states. For a spectral density peaked around 23 meV of width ~ 12 meV with maximum around 32 meV, as is indicated in tunnelling experiments, we find that a $T_c=95$ K can be obtained with a modest value of electron-boson mass renormalization parameter $\lambda=1.7$. This is to be compared with a value of 5.1 in an isotropic S-wave theory. In the D-wave-like case, a clear sharp peak is found at an energy which

would correspond to a gap to T_c ratio $2\Delta/k_BT_c$ of approximately 5.2, and the boson structure falls at an energy measured with this peak position taken to be the zero reference. At lower energies near $\omega=0$, $N_s(\omega)/N(0)$ is found to go towards zero almost linearly. This is in contrast to experiments of Valles *et al.*[4] in which a large zero bias current is observed. A finite value of $N_s(\omega)/N(0)$ at $\omega=0$ can easily be obtained by introducing in the theory impurity scattering in the strong scattering T-matrix limit with phase shift δ_0 near $\pi/2$ (unitary limit). The boson structure is not strongly affected by the introduction of such impurity scattering, and the curve for $N_s(\omega)/N(0)$ can be made to look very much like the measured curve at low ω, near the peak at the "gap" value, and in the boson region at higher energies. It should be stressed, however, that the band structure we have used is not very realistic for the specific case of $YBA_2Cu_3O_7$, which exhibits a more complex band structure and also contains chains as well as planes. The proximity of these chains can introduce complicated quasiparticle structure through the proximity effect.[35–37]

As temperature is increased towards T_c, thermal smearing is found to further fill the gap region near $\omega=0$ but the effects are small except near T_c. The amount of the filling is further increased as impurity scattering is increased. Temperature smearing is, of course, absent in BCS theory as is all boson structure at higher energies.

ACKNOWLEDGMENTS

We acknowledge a valuable discussion with David Pines and thank F. Marsiglio for reading the manuscript and pointing out a mistake. This work was supported, in part, by NSERC (Natural Sciences and Engineering Research Council of Canada), by CIAR (Canadian Institute for Advanced Research) and NSF-OMR 91-13631.

[1]W. L. McMillan and J. M. Rowell, in *Superconductivity,* edited by R. D. Parks (Marcel Dekker, New York, 1969), Vol. 1, p. 561.
[2]J. P. Carbotte, Rev. Mod. Phys. **62**, 1027 (1990).
[3]D. J. Scalapino, in *Superconductivity* (Ref. 1), Vol. 1, p. 449.
[4]J. M. Valles Jr., R. C. Dynes, A. M. Cucolo, M. Gurvitch, L. F. Schneemeyer, J. P. Garno, and J. V. Waszczak, Phys. Rev. B **44**, 11 986 (1991).
[5]P. Monthoux, A. Balatsky, and D. Pines, Phys. Rev. Lett. **67**, 3448 (1991).
[6]D. Pines, Physica C **185-189**, 120 (1991).
[7]C. T. Rieck, Th. Wölkhausen, D. Fay, and L. Tewordt, Phys. Rev. B **39**, 278 (1989).
[8]D. Pines, Physica B **163**, 78 (1990).
[9]S. Wermbter and L. Tewordt, Phys. Rev. B **44**, 9524 (1991).
[10]N. Bulut and D. J. Scalapino, Phys. Rev. Lett. **67**, 2898 (1991).
[11]A. J. Millis and H. Monien, Phys. Rev. B **45**, 3059 (1992).
[12]A. J. Millis, H. Monien, and D. Pines, Phys. Rev. B **42**, 167 (1990).
[13]A. J. Millis, S. Sachdev, and C. M. Varma, Phys. Rev. B **37**, 4975 (1988).
[14]M. Prohammer and J. P. Carbotte, Phys Rev. B **43**, 5370 (1991).
[15]P. J. Williams and J. P. Carbotte, Phys. Rev. B **39**, 2180 (1989).
[16]E. Schachinger and J. P. Carbotte, Phys. Rev. B **43**, 10 279 (1991).
[17]L. Coffey, T. M. Rice, and K. Ueda, J. Phys C **18**, L813 (1985).
[18]C. J. Pethick and D. Pines, Phys. Rev. Lett. **57**, 118 (1986).
[19]P. Hirschfeld, P. Wölfle, and D. Einzel, Phys. Rev. B **37**, 83 (1988).
[20]C. T. Rieck, D. Fay, and L. Tewordt, Phys. Rev. B **41**, 728 (1990).
[21]J. Keller, K. Scharnberg, and H. Monien, Physica C **152**, 302 (1988).
[22]H. Monien, K. Scharnberg, L. Tewordt, and D. Walker, Solid State Commun. **61**, 581 (1987).
[23]S. Schmitt-Rink, K. Miyake, and C. M. Varma, Phys. Rev. Lett. **57**, 2575 (1987).
[24]P. J. Hirschfeld, P. Wölfe, J. A. Sauls, D. Einzel, and W. O. Putikka, Phys. Rev. B **40**, 6695 (1989).
[25]R. A. Klemm, K. Scharnberg, D. Walker, and C. T. Rieck, Z. Phys. B **72**, 139 (1988).
[26]P. Hirschfeld, D. Vallhardt, and P. Wölfle, Solid State Commun. **59**, 111 (1986).
[27]F. Marsiglio, R. Akis, and J. P. Carbotte, Phys. Rev. B **45**, 9865 (1992).
[28]C. Jiang and J. P. Carbotte, Phys Rev. B **45**, 7368 (1992).
[29]C. Jiang and J. P. Carbotte, J. Low Temp. Phys. **87**, 95 (1992).
[30]F. Marsiglio, M. Schossmann, and J. P. Carbotte, Phys. Rev. B **37**, 4965 (1988).
[31]C. Jiang and J. P. Carbotte, Phys Rev. B **45**, 10 670 (1992).
[32]E. J. Nicol, C. Jiang, and J. P. Carbotte, Phys Rev. B (to be published).
[33]P. B. Allen and R. C. Dynes, Phys. Rev. B **12**, 905 (1975).
[34]H. J. Vidberg and J. W. Serene, J. Low Temp. Phys. **29**, 179 (1977).
[35]A. I. Buzdin, V. P. Damjanovic', and A. Yu Simonov, Physica C **194**, 109 (1992).
[36]A. I. Buzdin, V. P. Damjanovic', and A. Yu Simonov, Phys. Rev. B **45**, 7499 (1992).
[37]M. Tachiki, S. Takahashi, F. Steglich, and H. Adrian, Z. Phys. B **80**, 161 (1990).