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Energy gap, T_c, and density of states in high-temperature superconductors for retarded s- and d-wave interactions

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We employ strong-coupling theory to investigate the effect of the form of the spectral function α^2F for isotropic and anisotropic interactions on the tunneling density of states $N(\omega)$, T_c, and the ratio $2\Delta/k_BT_c$. Resistivity data are used to fix the isotropic coupling constant $\lambda_0 \sim 1$. This severely restricts the results for s-wave pairing; high-energy spectral weight is required in addition to phonons. The anisotropic interaction is not restricted by the resistivity and thus with d-wave pairing a variety of data, including the linear behavior of $N(\omega)$ within the gap, can be fitted without high-energy interactions.

Many measurements on high-T_c superconductors yield values for the ratio of the zero temperature gap 2Δ, to k_BT_c which are larger than the BCS weak-coupling value of 3.5. For example, recent tunneling data[1] give a value of approximately 4.1, while infrared data[2] and high-energy spectroscopy data[3] yield about 8. The gaplike feature seen in the tunneling conductance does not have the BCS shape and there is a finite value at zero bias which increases with T.[1] Other experiments, in particular Raman measurements,[4] also indicate the existence of electronic states extending below the gap. The latter experiments have been explained by assuming a d-wave pair state which has nodes within the superconducting gap.[5] However, for d-wave pairing, weak-coupling theory yields a ratio $2\Delta/k_BT_c$ which is *smaller* than the BCS value.[6] Here Δ is the average over the Fermi surface.

The conditions under which the retarded interaction of the Eliashberg theory can yield large values of $2\Delta/k_BT_c$ have been studied extensively for s-wave[7] as well as for d-wave superconductivity.[8] In view of the new experiments on high-T_c superconductors it seems necessary to reexamine the previous conventional strong-coupling theories. Generally, one finds that a large ratio is strongly correlated with a large value of the mass enhancement parameter λ_0 (s-wave coupling parameter). Here we investigate the size of the ratio and the possibility of obtaining $T_c \simeq 100$ K under the assumption that λ_0 is relatively small, $\lambda_0 \lesssim 1$. Later we employ resistivity measurements to give some justification for this assumption. This assumption leads to restrictions on the possible pair states and pairing mechanisms. We now find that, with reasonable assumptions for the spectral function of the strong-coupling theory α^2F, it does not seem possible to obtain a ratio as large as 8. The parameter values suggested by Ref. 1 ($T_c = 90$ K, $2\Delta/k_BT_c = 4.1$) can be fitted for $\lambda_0 = 0.8$ with a phonon-mediated pairing interaction in the anisotropic, d-wave case. In order to fit these data for s-wave pairing, we require, in addition to the phonons, spectral weight at higher frequencies > 100 meV, arising perhaps from exchange of excitons or spin fluctuations. In the isotropic case we of course do not find the observed states within the gap.[1]

Our starting point is the well-known generalized Eliashberg equations[9] for the renormalization function $Z(\mathbf{k}, i\omega_n)$, the energy shift $\chi(\mathbf{k}, i\omega_n)$, and the order parameter $\Phi(\mathbf{k}, i\omega_n)$ whose kernels depend on the retarded interaction $\alpha^2F(\mathbf{k},\mathbf{k}';\Omega)$, the Coulomb interaction $\mu^*(\mathbf{k},\mathbf{k}')$, and the effective band ϵ_k. Here we assume for simplicity that $\mathbf{k}$ and $\mathbf{k}'$ lie in the a-b plane (CuO_2 plane). Thus we neglect the relatively small band dispersion and the gap in the c direction. The solutions of the full equations for a tight-binding band[10] show that the Green's functions are sharply peaked at the Fermi surface. Thus it is a good approximation to integrate over ϵ_k normal to the Fermi surface from $-\infty$ to $+\infty$. For small band fillings where the Fermi line is nearly a circle, the Eliashberg equations become approximately [ϕ is the azimuthal angle of $\mathbf{k}$ in the a-b plane, $\Delta(i\omega_n) = \Phi(i\omega_n)/Z(i\omega_n)$ is the gap function]

$$\omega_n[Z(\phi,i\omega_n)-1] = \pi T \sum_{m=-\infty}^{+\infty} \int_0^{2\pi} \frac{d\phi'}{2\pi} \lambda(\phi,\phi';n-m)\omega_m[\omega_m^2+\Delta^2(\phi',i\omega_m)]^{-1/2}, \tag{1}$$

$$\Delta(\phi,i\omega_n)Z(\phi,i\omega_n) = \pi T \sum_{m=-\infty}^{+\infty} \int_0^{2\pi} \frac{d\phi'}{2\pi} [\lambda(\phi,\phi';n-m)-\mu^*(\phi,\phi')\theta(\omega_c-|\omega_m|)]\Delta(\phi',i\omega_m)[\omega_m^2+\Delta^2(\phi',i\omega_m)]^{-1/2}, \tag{2}$$

$$\lambda(\phi,\phi';n-m) = \int_0^{\infty} d\Omega\, \alpha^2F(\phi,\phi';\Omega)2\Omega(\omega_{n-m}^2+\Omega^2)^{-1}. \tag{3}$$

We expand α^2F and μ^* in terms of basis functions $\psi_i(\phi)$ where the first few functions of lowest order are

$$\psi_0 = 1; \quad \psi_1(\phi) = \sqrt{2}\cos(2\phi); \quad \psi_2(\phi) = \sqrt{2}\sin(2\phi). \tag{4}$$

The d-wave functions ψ_1 and ψ_2 have Γ_3^+ and Γ_4^+ symmetry.[11] We study here the following model interaction:

$$\alpha^2F(\phi,\phi';\Omega) = \alpha^2F_{00}(\Omega)+\alpha^2F_{11}(\Omega)\psi_1(\phi)\psi_1(\phi'). \tag{5}$$

Equation (3) then yields an analogous expansion for the interaction kernel $\lambda(\phi,\phi';n-m)$ with components

$$\lambda_{ii}(n-m)=\int_0^\infty d\Omega\,\alpha^2F_{ii}(\Omega)2\Omega(\omega_{n-m}^2+\Omega^2)^{-1} \quad (6)$$

$$(i=0,1).$$

Note that Eq. (5) is invariant under rotation by $\pi/2$. For the isotropic and anisotropic spectral functions $\alpha^2F_{ii}(\Omega)$, $(i=0,1)$, we have taken δ function or Lorentzian peaks at different frequencies with different weights. The coupling strengths λ_i are defined by $\lambda_i=\lambda_{ii}(0)$.

We have solved numerically the system of coupled equations (1) and (2) with kernels given by Eqs. (3)–(6). To a good approximation we find that $Z(\phi,i\omega_n)$ is always independent of ϕ and that $\Delta(\phi,i\omega_n)$ is either purely s wave or purely d wave. The region of stability of the two types of solutions depends on the relative positions and strengths of the peaks in α^2F_{ii}; in general, the stable solution is the one corresponding to the peak with greater strength and/or higher frequency. If both peaks have comparable strength and position, the choice of trial solution determines the solution to which the iteration procedure converges.

We first consider d-wave pairing. Consistent solutions are obtained by setting $Z=Z_0(i\omega_n)$ and $\Delta=\Delta_1(i\omega_n)\times\psi_1(\phi)$. The results for $\Delta_2(i\omega_n)\psi_2(\phi)$ are identical. Inserting these expansions together with Eqs. (3)–(6) into Eqs. (1) and (2), Eq. (1) becomes a set of equations for $Z_0(i\omega_n)$ containing the isotropic interaction $\lambda_{00}(n-m)$ and Eq. (2) becomes a set of equations for $\Delta_1(i\omega_n)$ containing the anisotropic interaction $[\lambda_{11}(n-m)-\mu_{11}^*]\times\psi_1^2(\phi')$. The gap function $\Delta_1(\omega)$ is obtained from $\Delta_1(i\omega_n)$ by the analytic continuation $i\omega_n\rightarrow\omega+i0^+$ with the method of Padé approximants. The average of the magnitude of the gap is given by $\Delta_1=\mathrm{Re}[\Delta_1(\Delta_1)]$. We calculate the tunneling density of states from

$$\frac{N(\omega)}{N_0}=\int_0^{2\pi}\frac{d\phi}{2\pi}\mathrm{Re}\{\omega[\omega^2-\Delta_1^2(\omega)\psi_1^2(\phi)]^{-1/2}\}. \quad (7)$$

Note that our procedure differs from that of Ref. 8 where only the anisotropic part and not the coupled equations was considered. Also, the **k** dependence of the gap function appearing within the square root in Eqs. (1) and (2) was neglected there, which could adversely affect their results far below T_c.

One of our primary goals is to investigate how well the theory can reproduce the measured tunneling conductance $G(V)$ for $YBa_2Cu_3O_7$/Pb junctions.[1] At low temperature $G(V)$ rises almost linearly with V from a zero-bias value (the feature at 4 meV is attributed to Δ_c which is neglected here). The reason that the zero-bias value is finite and increases with T is not yet known. At 19 meV a peak occurs which is attributed to the $\Delta_{a\text{-}b}$ gap. A second peak occurs at 36 meV followed by a minimum near 49 meV. The sharp decrease around 42 meV is thought to arise from a phonon peak in α^2F at about $\Omega_0=23$ meV, since $\Delta_{a\text{-}b}+\Omega_0=42$ meV. We have thus assumed an isotropic peak in α^2F_{00} at $\Omega_0=23$ meV with a coupling strength somewhat arbitrarily fixed at $\lambda_0=0.8$. For simplicity we always assume $\mu^*=0$. In Fig. 1 we shown $N(\omega)$ for the case of the anisotropic peak at $\Omega_1=30$ meV with $\lambda_1=1.33$

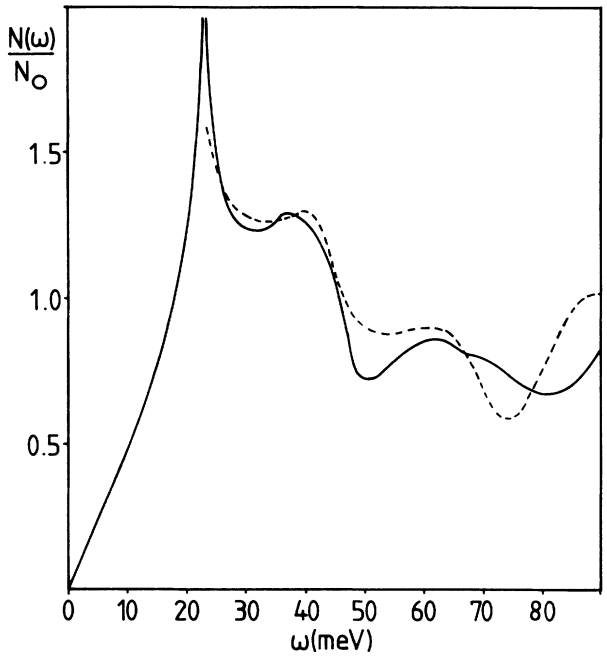

FIG. 1. Tunneling density of states for d-wave pairing with parameters $\lambda_0=0.8$, $\lambda_1=1.33$, $\Omega_0=23$ meV, $\Omega_1=30$ meV, $T=10$ K, $T_c=89.6$ K, $\mu^*=0$, and $2\Delta_1/k_BT_c=4.16$. Solid curve: δ-function peaks in α^2F. Dashed curve: Lorentz peaks with half-width 14 meV.

which yields $T_c=89.6$ K, $\Delta_1=16.08$ meV, and $2\Delta_1/k_BT_c=4.16$. $N(\omega)$ is accurately linear for small ω and a first peak occurs at $\sqrt{2}\Delta_1=23$ meV corresponding to the amplitude of the d-state gap. By examining Eq. (7) for $N(\omega)$ one can easily verify that $N(\omega)\simeq\omega/\mathrm{Re}\Delta_1$ for $\omega\rightarrow 0$, and that $N(\omega)$ diverges logarithmically for ω approaching the gap edge from below. A second peak occurs in Fig. 1 at about 37 meV. This peak arises primarily from the peak in α^2F_{11} as can be seen by varying Ω_1 and λ_1. Both peaks in α^2F have been taken as δ functions. Except for a little smoothing of the phonon peak, finite-width peaks in α^2F lead to only minor changes in the detailed structure of $N(\omega)$, as seen in Fig. 1.

In Fig. 2 we show the dependence of the ratio $2\Delta_1/k_BT_c$ on the position Ω_1 of the anisotropic peak for constant isotropic peak. Also shown is the value of λ_1 required to maintain $T_c=90$ K. We see that, if one wants a large ratio, there is an "optimum" value of Ω_1 at about 40 meV which depends on T_c but not on Ω_0 or λ_0. The value of the ratio at maximum, however, increases with decreasing Ω_0, but it does not seem possible to get ratios much above 4.5. Note that ratios less than 3.5 can occur for large Ω_1. Below about 30 meV, Δ_1 decreases as $(\lambda_1)^{1/2}\Omega_1$. It is interesting that the isotropic peak tends to be pair breaking in the sense that increasing λ_0 with Ω_0 constant requires an *increase* in λ_1 to maintain constant T_c. This could lead to a reduced isotope effect.

We turn now to the isotropic solutions of Eqs. (1) and (2) which are stable for $\lambda_0>\lambda_1$. A consistent solution is obtained by setting $Z=Z_0(i\omega_n)$ and $\Delta=\Delta_0(i\omega_n)$. Equations (1) and (2) then reduce to the standard isotropic

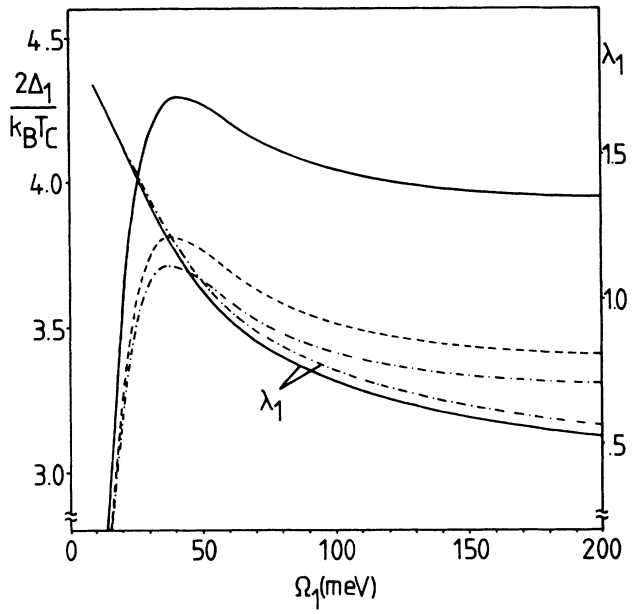

FIG. 2. Anisotropic ratio $2\Delta_1/k_BT_c$ and pairing parameter λ_1 vs anisotropic peak frequency Ω_1 for $\lambda_0=0.8$ and $\Omega_0=23$ meV (solid), 50 meV (dashed), and 70 meV (dot-dashed). $T=10$ K and $T_c=90$ K. The λ_1 curves for $\Omega_0=50$ and 70 meV are indistinguishable.

Eliashberg equations. We have investigated several possibilities for α^2F to see if the conditions $\lambda\simeq 1$, $2\Delta/k_BT_c\simeq 4$ and $T_c\simeq 90$ K can be fulfilled simultaneously: (a) "Phonon" peaks alone; (b) "phonon" plus "exciton"; (c) "phonon" plus negative μ^*. In case (a) we consider typical phonon spectra in the frequency range below 100 meV. For example, a single peak in α^2F at 30 meV with a half-width of 20 meV yields the expected structure in $N(\omega)$ but $\lambda=2.9$ and $2\Delta/k_BT_c=5.9$ are much too large. With two peaks at 20 and 70 meV we can only come close to fulfilling the conditions when almost all the spectral weight is in the upper peak. Then the structure in $N(\omega)$ near 40 meV disappears. The condition $\lambda\simeq 1$ severely restricts the possibilities: We cannot then obtain T_c as large as 90 K with a reasonable phonon spectrum and we conclude that isotropic phonons alone are not sufficient. A number of experiments, however, e.g., thermal conductivity measurements, give strong evidence that the electron-phonon interaction does play an important role in high-T_c materials. The coupling strength, at least for acoustic phonons, seems, however, to be relatively small.[12] In case (b) we thus assume a phonon peak in α^2F of half-width 15 meV centered at 23 meV as indicated in Ref. 1. This peak alone yields $\lambda_{ph}=0.8$, $T_c=21$ K, and $2\Delta/k_BT_c=3.98$. A δ-function exciton (which could be a spin fluctuation or other type of excitation) peak is then placed at Ω_e with strength λ_e adjusted to yield $T_c=90$ K. The results for several values of Ω_e are shown in Table I. It is seen that the conditions $\lambda_e+\lambda_{ph}\simeq 1$ and a ratio of 4 require an exciton peak at a frequency above 100 meV. $N(\omega)$ shows the expected structure due to the phonons and exciton although the phonon structure is rather weak for $\omega_e>100$ meV.

TABLE I. "Exciton" coupling parameter λ_e and the ratio $2\Delta/k_BT_c$ for various exciton frequencies. $T_c=90$ K and $\lambda_{ph}=0.8$ in all cases.

Ω_e (meV)	λ_e	$2\Delta/k_BT_c$
30	2.20	5.98
70	0.80	4.84
200	0.42	4.55
300	0.35	4.53

For completeness we have considered the above phonon but replaced the exciton peak with a negative μ^*. A μ^* of -0.2 yields the same results as the exciton peak at 200 meV. A peak in α^2F, however, seems to be a more plausible representation of the likely nonphonon mechanisms.

It is interesting that the ratio $2\Delta/k_BT_c$ for the phonon plus exciton together is larger than for either the phonon alone or the exciton alone. The exciton at 200 meV alone gives $T_c=60$ K and a ratio of 3.74. Together with the phonon at 23 meV, Table I shows a ratio of 4.55 while the phonon alone gave 3.98. An exciton at 200 meV with $\lambda_e=0.496$ yields $T_c=90$ K and a ratio of 3.8. It is thus possible for the nonphonon part of α^2F to be responsible for the high T_c while the phonons produce structure in $N(\omega)$ and both mechanisms together raise $2\Delta/k_BT_c$ significantly above the BCS value. Apparently a low-lying phonon has an enhanced pair-breaking effect in the presence of the high-energy excitation. A similar effect was found in Ref. 8 but only in the anisotropic case. That an exciton alone at 200 meV yields a ratio 3.8 may seem surprising in view of the fact that $T_c/\Omega_e=0.04$. We point out that in BCS (i.e., a constant interaction $\lambda=N_0V$ and cutoff ω_c), while the weak-coupling limit $\lambda\ll 1$ gives the well-known ratio of 3.53, the limit $\lambda\gg 1$ yields a ratio of 4. It is thus possible in BCS, even for rather small T_c/ω_c, to obtain, with $\lambda\simeq 1$, a ratio greater than 3.5.

We now consider the justification for taking $\lambda_0=0.8$. This is important since, within the conventional isotropic strong-coupling theory, it is relatively easy to obtain a T_c of 100 K and a ratio of 8 (or more), if one assumes strong enough phonons which yield a large λ_0. A major objection to this procedure is that such phonons should have a significant effect on the normal-state resistivity $\rho(T)$. To investigate this point we use Ziman's resistivity formula[13]

$$\rho(T)\simeq\frac{4\pi m}{ne^2k_BT}\int_0^{\omega_{\max}}d\omega\frac{\hbar\omega\alpha_{\rm tr}^2F(\omega)}{[\exp(\hbar\omega/k_BT)-1][1-\exp(-\hbar\omega/k_BT)]}, \tag{8}$$

where the transport coupling function is defined as

$$\alpha_{\rm tr}^2F(\omega)=\int_{FS}d^2k_F\,n(\mathbf{k}_F)d^2k_F'\,n(\mathbf{k}_F')\alpha^2F(\mathbf{k},\mathbf{k}',\omega)\left[1-\frac{\mathbf{v}_k\cdot\mathbf{v}_{k'}}{|\mathbf{v}_k|^2}\right]. \tag{9}$$

Here $n(k_F)$ is the normalized density of states. Evaluating Eq. (8) in the present model we find that the anisotropic part of the interaction, Eq. (5), does not contribute and is thus not restricted by the resistivity. Inserting the isotropic peak used in Fig. 1, $\rho(T)$ is linear up to $T \simeq 1000$ K. Values of 1.0–1.2 eV for the plasma frequency[14] and 50–200 $\mu\Omega$ cm for $\rho(T_c)$ (Ref. 15) yield $\lambda_0 \simeq 0.3$–1.4. Thus the chosen value of $\lambda_0 = 0.8$ seems to be, at least, consistent. To pose more restrictive bounds on λ_0, measurements of ω_{p1} and $\rho(T)$ on the same sample would be extremely useful. Thus, a small value of λ from electrical and thermal conductivity measurements does not necessarily mean that the anisotropic part of the electron-phonon interaction is small.

In conclusion we can say that it seems feasible that Eliashberg theory can account for high-T_c superconductivity if the isotropic electron-phonon interaction of modest strength is supplemented by some other kind of mechanism. For s-wave pairing we have obtained values of $2\Delta/k_BT_c$ as large as about 5 by adding to the phonon peak an exciton peak in the spectral function of the isotropic interaction. The resulting density of states can show reasonable structure above the gap but of course does not show the almost linear behavior at low frequency observed in the tunneling conductance of $YBa_2Cu_3O_7$/Pb junctions.[1]

Anisotropic gaps, like our d-wave Δ_1, can be found if the retarded interaction contains a substantial amount of d-wave component. This could arise from phonons, spin fluctuations, or excitons, for example. We have seen that one can easily obtain ratios $2\Delta/k_BT_c$ of 4 which are in accordance with Ref. 1. We stress again that weak-coupling theory[6] yields a value of this ratio for a d-wave state which is *smaller* than the BCS s-wave value of 3.5. Thus, an anisotropic ratio of 4 corresponds to rather strong coupling. The density of states $N(\omega)$ seems to fit the tunnel measurements somewhat better for d-wave than for s-wave pairing, especially the linear behavior for small ω within the gap. This linear behavior of $N(\omega)$ is obviously due to the four point nodes in the two-dimensional gap. This is different from the three-dimensional case where point nodes in the gap lead to ω^2 behavior of $N(\omega)$. A line of nodes, however, leads to $N(\omega) \propto \omega$.[16]

The following point is worth mentioning: In strong-coupling theory one very often simulates a peak in α^2F with a δ function. This is quite satisfactory for determining the ratio $2\Delta/k_BT_c$, for example. One must be careful in computing quantities like $N(\omega)$ that depend on detailed structure of the gap function. In the isotropic case the δ function produced extraneous structure in $N(\omega)$.

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