

Strong coupling to multiple phonon modes in high-temperature superconductors

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The spectra of the second derivative of tunneling current d^2I/dV^2 in the high-temperature superconductors $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ and $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ show clear dip and peak features due to strong coupling to the bosonic modes mediating electron pairing. The energy positions of nearly all the peaks in $-d^2I/dV^2$ -like spectra match precisely with those in the phonon density of states obtained by inelastic neutron scattering. The results demonstrate that the bosonic modes mediating the electron pairing are phonons and that high-temperature superconductivity arises primarily from strong coupling to multiple phonon modes.

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The identification of phonon anomalies in the tunneling spectra¹ and the observation of an isotope effect² provide important and crucial clues to the understanding of the microscopic pairing mechanism of superconductivity³ in conventional metals. For high-transition-temperature (high- T_c) copper oxide superconductors, extensive studies of various unconventional oxygen-isotope effects have clearly shown strong electron-phonon interactions and the existence of polarons.⁴⁻¹⁵ Neutron scattering,¹⁶ angle-resolved photoemission (ARPES),¹⁷ and Raman scattering¹⁸ experiments also provide evidence for the strong electron-phonon coupling. However, these experiments do not provide direct evidence that pairing is predominantly mediated by phonons. Recent ARPES data concerning the effects of electron-boson interactions on electron self-energies have led to contradictory conclusions. On one hand, in the diagonal direction of momentum space (π, π) , the observed “kink” features around 70 meV in the band dispersion of several cuprate compounds appear to provide evidence for strong coupling between electrons and the 70 meV Cu-O half-breathing mode.¹⁹ The coupling to this 70 meV phonon mode is shown to be primarily responsible for d -wave high- T_c superconductivity.²⁰ On the other hand, Devereaux *et al.* propose that the 36 meV B_{1g} Cu-O buckling mode rather than the 70 meV mode is the main player for d -wave high- T_c superconductivity based on ARPES data near the antinodal direction.²¹ To further complicate matters, a third group²² has even provided a completely different interpretation for the ARPES data in the antinodal direction, that is, the kink feature is related to a magnetic resonance mode rather than a phonon mode. It is clear that the identity for the bosonic modes mediating the electron pairing is inconclusive due to these contradictory interpretations.

In order to unambiguously identify the origin of the bosonic modes mediating the electron pairing, it is essential to precisely determine the energies of the bosonic modes. If the energies of the bosonic modes have a one-to-one correspondence to the energies of the peak positions in the phonon density of states determined from inelastic neutron scattering, one can definitively conclude that phonons predominantly mediate the pairing. For conventional superconductors, strong electron-phonon coupling features clearly show up in single-particle tunneling spectra.^{1,23} The energies of the phonon modes coupled to electrons can be precisely deter-

mined from tunneling spectra. More specifically, the energy positions of the peaks in $-d^2I/dV^2$, measured from the isotropic s -wave superconducting gap Δ , correspond to those of the peaks in the electron-phonon spectral function $\alpha^2(\omega)F(\omega)$ (Refs. 1 and 23). Therefore, if the coupling strength $\alpha^2(\omega)$ does not have pronounced structures, the structures in the phonon density of states $F(\omega)$ will have a one-to-one correspondence to those in $-d^2I/dV^2$. Such a conventional approach to identify the electron-boson coupling features would have been extensively applied to high- T_c superconductors if the superconducting gap were isotropic. Since the superconducting gap is highly anisotropic in high- T_c superconductors, it is difficult to reliably determine the energies of bosonic modes if tunneling current is not directional. This may explain why the electron-boson coupling structures extracted from earlier tunneling spectra are not reproducible among different groups.²⁴⁻²⁶ In a very recent article²⁷ attempting to show an important role of phonons in the electron pairing, the authors assign the energy (52 meV) of a peak position in $+d^2I/dV^2$ spectra of $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ to the energy of a phonon mode. Such an assignment is incorrect because the energies of phonon modes are equal to the energies of dip positions rather than peak positions in $+d^2I/dV^2$ (Refs. 1 and 23).

Here, we report d^2I/dV^2 -like spectra for the high- T_c superconductors $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ (YBCO) and $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ (BSCCO). We find that the energy positions of nearly all the peaks in d^2I/dV^2 -like spectra match precisely with those of the peaks in the phonon density of states obtained by inelastic neutron scattering. Such excellent agreement between tunneling and neutron data can be explained only if the tunneling currents in these junctions are highly directional and the phonon modes primarily contribute to the electron pairing.

Figure 1(a) shows the normalized scanning tunneling microscopic (STM) conductance spectrum $g_{NM} = (dI/dV)/(dI/dV)_B$ at 4.2 K for a slightly overdoped YBCO with $T_c = 90$ K, where $(dI/dV)_B$ is the background conductance at high biases. The data are taken from Ref. 28 and the normalized conductance is enlarged by a factor of 1.06 to ensure unity at high biases. The spectrum shows negligible zero-bias conductance and sharp peak at $eV = 19.6$ meV, suggesting that the superconducting gap Δ is about 19.6 meV. The solid red line is the BCS density of states: N_{BCS}

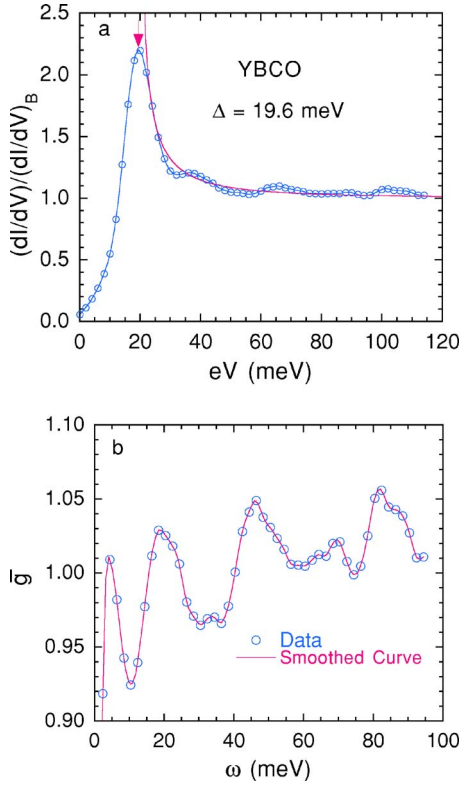


FIG. 1. (Color online) (a) Normalized STM conductance $g_{NM}=(dI/dV)/(dI/dV)_B$ versus energy $E=eV$ for a slightly overdoped $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ (YBCO) with $T_c=90$ K, where $(dI/dV)_B$ is the background conductance at high biases. The STM conductance spectrum was taken on the (001) crystal face with a Pt-Ir tip at 4.2 K (Ref. 28). (b) The renormalized conductance $\bar{g}=g_{NM}/N_{BCS}$ versus $\omega=eV-\Delta$ (the energy measured from the gap Δ) for $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$. The solid line is a smoothed curve obtained using a cubic-spline interpolation.

$=eV/\sqrt{(eV)^2-\Delta^2}$, which lies in the middle of the data points. In Fig. 1(b), we plot renormalized conductance $\bar{g}=g_{NM}/N_{BCS}$ versus $\omega=eV-\Delta$ (the energy measured from the gap). After the renormalization, the structures due to strong electron-boson coupling can be clearly seen in the first derivative spectrum of tunneling current.

In order to precisely determine the energies of the bosonic modes coupled to electrons, it is essential to take the derivative of the renormalized conductance \bar{g} . In Fig. 2(a), we show the $-\Delta(d\bar{g}/d\omega)$ spectrum of the YBCO crystal together with the phonon density of states $F(\omega)$ obtained by inelastic neutron scattering.²⁹ For comparison, in Fig. 2(b) we show the $-\Delta(d\bar{g}/d\omega)$ spectrum and $F(\omega)$ for the conventional phonon-mediated superconductor Pb. It is apparent that the $-\Delta(d\bar{g}/d\omega)$ spectra for both YBCO and Pb show peak, dip, or shoulder features. A single broad peak or shoulder in $F(\omega)$ and $-\Delta(d\bar{g}/d\omega)$ can occur when the separations of multiple peak features are too small compared to their widths. For Pb, nearly all the peaks and/or shoulder features in $-\Delta(d\bar{g}/d\omega)$ match precisely with those in $F(\omega)$, as expected from the phonon-mediated pairing mechanism. However, the peaks at 3.3 meV and 8.9 meV in the phonon density of states correspond to the dips in the tunneling spectrum. This mismatch is

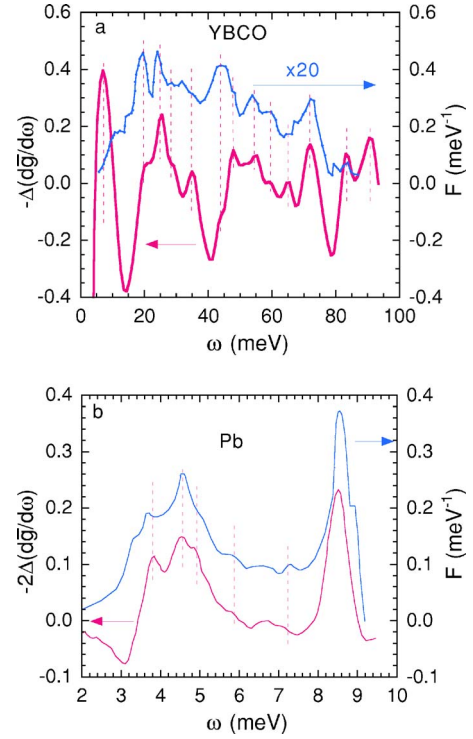


FIG. 2. (Color online) (a) $-\Delta(d\bar{g}/d\omega)$ spectrum for the $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ crystal together with the phonon density of states $F(\omega)$ obtained from inelastic neutron scattering (Ref. 29). The left scale is for $-\Delta(d\bar{g}/d\omega)$ and the right scale is for $F(\omega)$. The vertical dashed lines mark peak and/or shoulder features in $-\Delta(d\bar{g}/d\omega)$. (b) $-2\Delta(d\bar{g}/d\omega)$ spectrum together with the phonon density of states $F(\omega)$ for the conventional phonon-mediated superconductor Pb. Here, $\bar{g}=N_s/(N_n N_{BCS})$, N_s is the superconducting density of states, and N_n is the density of states in the normal state. The left scale is for $-2\Delta(d\bar{g}/d\omega)$ and the right scale is for $F(\omega)$. The data of N_s/N_n are from Ref. 1, and the data of $F(\omega)$ are from Ref. 30. The vertical dashed lines mark peak and/or shoulder features in $-\Delta(d\bar{g}/d\omega)$.

due to the fact that the coupling strengths for the two modes are much weaker.

If strong coupling to phonon modes also happens in high- T_c superconductors such as YBCO, then the peak and/or shoulder features in $-\Delta(d\bar{g}/d\omega)$ should line up with the peak and/or shoulder features in the phonon density of states as well. Indeed, nearly all 13 peak and/or shoulder features in $-\Delta(d\bar{g}/d\omega)$ of YBCO match precisely with those in $F(\omega)$. The strong coupling features at 7.1 and 90.8 meV in $-\Delta(d\bar{g}/d\omega)$ cannot compare with these neutron data since the energy positions of these features are outside the energy range of the neutron data. Nevertheless, the phonon peak at about 6.8 meV is clearly seen in the high-resolution neutron data of BSCCO [see Fig. 3(a)]. The feature at 90.8 meV should be the composite phonon energy of 7.1 and 83.7 meV since the sum of 7.1 and 83.7 meV is equal to 90.8 meV. This is expected from the conventional strong-coupling theory.^{1,23} Such excellent agreement between neutron and tunneling data provides clear evidence that the bosonic modes mediating the electron pairing are phonons and that the tunneling current of this junction is highly directional.

It is interesting that the low-energy modes at 7.1, 20.3,

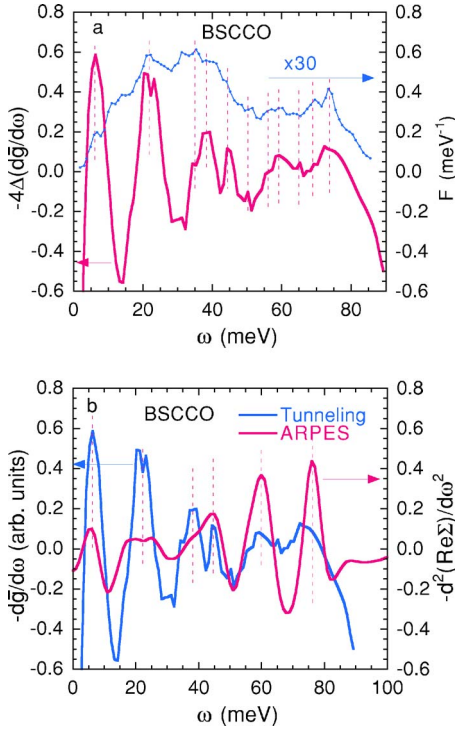


FIG. 3. (Color online) (a) $-\Delta(d\bar{g}/d\omega)$ spectrum for a $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ crystal with $T_c=93$ K and the phonon density of states $F(\omega)$ at 296 K. The high-resolution neutron data of $F(\omega)$ are reproduced from Fig. 1(a) of Ref. 31. The left scale is for $-4\Delta(d\bar{g}/d\omega)$ and the right scale is for $F(\omega)$. The vertical dashed lines mark peak and/or shoulder features in $-4\Delta(d\bar{g}/d\omega)$. (b) The $-d^2(\text{Re}\Sigma)/d\omega^2$ spectrum (Σ is electron self-energy) (Ref. 32) and the $-d\bar{g}/d\omega$ tunneling spectrum of BSCCO crystal. The $-d^2(\text{Re}\Sigma)/d\omega^2$ spectrum is reproduced from Ref. 32. Vertical dashed lines mark the peak positions in the $-d^2(\text{Re}\Sigma)/d\omega^2$ spectrum.

and 25.5 meV have much stronger coupling than the higher energy modes and thus contribute more to the electron pairing. In contrast, the electron-phonon coupling strengths for the 14.6 and 31.9 meV phonon modes are much weaker because the dip features in $-\Delta(d\bar{g}/d\omega)$ occur at these phonon energies.

If the strong electron-phonon coupling features in YBCO are intrinsic, they should also show up in other 90 K superconductors. In Fig. 3(a), we show the $-\Delta(d\bar{g}/d\omega)$ spectrum for a BSCCO crystal together with the phonon density of states $F(\omega)$ at 296 K. Here, $\bar{g}=N_s(\omega)/[N_n(\omega)N_A(\omega)]$ and $N_A(\omega)$ is a smoothed curve of $N_s(\omega)/N_n(\omega)$, which is proportional to $1+0.99\exp(-\omega/18.7)+0.13\exp[-(\omega-71.3)^2/779]$ and does not have fine structures. The data of $N_s(eV)/N_n(eV)$ are obtained from Fig. 5(a) of Ref. 26. The $N_s(eV)/N_n(eV)$ spectrum has a peak at $eV=25.2$ meV (Ref. 26), suggesting $\Delta\approx 25.2$ meV. This gap size is smaller than the average gap expected for a BSCCO with $T_c=93$ K. Thus, the spectrum may be probing a higher

doping region with $T_c\approx 89$ K in the intrinsically inhomogeneous BSCCO.

From Fig. 3(a), we can clearly see that nearly all the peak and/or shoulder features in the $-\Delta(d\bar{g}/d\omega)$ spectrum match precisely with those in the room-temperature phonon density of states. The peak feature at 65.0 meV in $-\Delta(d\bar{g}/d\omega)$ is slightly off from the peak at 64.0 meV in the room-temperature neutron data. It is interesting to note that two peaks at 14.4 meV and 31.8 meV in the phonon density of states correspond to the dips in the tunneling spectrum. For YBCO, this mismatch occurs at 14.6 meV and 31.9 meV [see Fig. 2(a)], which are very close to those (14.4 and 31.8 meV) for BSCCO. Such quantitative agreement indicates that the 14 and 32 meV phonon modes in both YBCO and BSCCO have much weaker coupling to electrons.

In Fig. 3(b), we compare the strong coupling features revealed in the tunneling spectrum and in the electron self-energy spectrum of BSCCO. The spectrum of the second derivative of the real part of electron self-energy $-d^2(\text{Re}\Sigma)/d\omega^2$ is reproduced from Ref. 32. It is striking that the peak features in $-d^2(\text{Re}\Sigma)/d\omega^2$ match very well with those in $-d\bar{g}/d\omega$. This excellent agreement between the tunneling and self-energy spectra further demonstrates that the observed strong-coupling features in both spectra are intrinsic.

It is known that any bosonic modes that mediate the electron pairing show up in tunneling spectra. The present tunneling spectra of both YBCO and BSCCO clearly demonstrate that the bosonic modes below 100 meV, which contribute to the electron pairing, are only the phonon modes. On the other hand, pairing mechanisms based on strong coupling to a magnetic resonance mode predict a pronounced dip feature at about 40 meV in the $dI/d\omega$ spectra of 90 K superconductors.³³ In contrast, the dip feature is found to occur at about 26 meV, which is nearly independent of doping.²⁷ This suggests that the dip feature is not caused by strong coupling to the magnetic mode. Moreover, the observed large reduced gap ($2\Delta/k_B T_c > 5$) implies a large coupling constant (> 2) and a quite low logarithmic mean boson energy $\hbar\omega_{\text{ln}} (< 40$ meV).²³ This rules out pairing mechanisms based on strong coupling to high-energy magnetic and/or charge excitations. Therefore, these tunneling spectra indicate that high-temperature superconductivity should arise primarily from strong coupling to multiple phonon modes.

In summary, we have shown that the energy positions of nearly all the peaks in $-d^2I/dV^2$ -like spectra of $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ and $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ match precisely with those of the peaks in the phonon density of states obtained by inelastic neutron scattering. The results demonstrate that the bosonic modes mediating the electron pairing are phonons and that high-temperature superconductivity should arise primarily from strong coupling to multiple phonon modes. The identification of an extended s -wave gap symmetry in the bulk³⁴ supports the phonon-mediated pairing mechanism.

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