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Precise determination of the superconducting gap along the diagonal direction of $Bi_2Sr_2CaCu_2O_{8+y}$: Evidence for an extended *s*-wave gap symmetry

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We report high-resolution spectra of the second derivative $-d^2(\mathrm{Re}\,\Sigma)/d\omega^2$ of the real part of electron self-energy Σ along the diagonal direction (where $\omega=E_F-E-\Delta_D$ and Δ_D is the diagonal superconducting gap) for a nonsuperconducting $La_{1.97}Sr_{0.03}CuO_4$ (LSCO) crystal and a superconducting $Bi_2Sr_2CaCu_2O_{8+y}$ (BSCCO) crystal with $T_c=91$ K. The $-d^2(\mathrm{Re}\,\Sigma)/d\omega^2$ spectrum of the nonsuperconducting LSCO shows clear peak features, which match precisely with those in the phonon density of states obtained from neutron scattering. Similarly, if we assign $\Delta_D=7\pm1$ meV for the superconducting BSCCO, the peak features in $-d^2(\mathrm{Re}\,\Sigma)/d\omega^2$ of this compound also match precisely with those in the phonon density of states and the tunneling spectrum. The present results rule out seemingly well accepted *d*-wave gap symmetry and strongly support an extended *s*-wave gap symmetry with eight line nodes.

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The phenomenon of superconductivity involves the pairing of electrons into Cooper pairs.[1] The internal wave function (gap function) of these Cooper pairs obeys a certain symmetry which reflects the underlying pairing mechanism. It is known that conventional superconductors (e.g., Pb and Nb) possess an *s*-wave gap symmetry that reflects the phonon mediated electron pairing.[1] On the other hand, the symmetry of the gap function in high-temperature superconductors has been a topic of intense debate for over fifteen years. Phase-sensitive experiments based on planar Josephson tunneling[2] appear to provide compelling evidence for *d*-wave order parameter (OP) symmetry. Since the gap symmetry is the same as the OP symmetry in BCS-like superconductors, these experiments lead to a widespread belief that *d*-wave gap symmetry has been firmly established for high-temperature superconductors. However, it is worth noting that these phase-sensitive experiments are probing the OP symmetry on surfaces or interfaces, which are found to be significantly underdoped.[3,4] The evidence for *d*-wave OP symmetry on the underdoped surfaces or interfaces is consistent with *d*-wave symmetry of the Bose-Einstein condensate of intersite oxygen-hole pairs,[5] which are the primary charge carriers in underdoped cuprates.[6] Therefore, these surface- and phase-sensitive experiments do not provide conclusive evidence for *d*-wave gap symmetry in the bulk of high-temperature superconductors.

On the other hand, several independent bulk-sensitive experiments (e.g., penetration depth and thermal conductivity measurements) have pointed to the existence of line nodes in the gap function.[7–10] Qualitatively, these experiments are consistent with *d*-wave gap function with four line nodes. Nevertheless, these data are also consistent with an extended *s*-wave gap function (*s*+*g* wave), which has eight line nodes when the *g*-wave component is larger than the *s*-wave one. Therefore, either *d*-wave or extended *s*-wave gap symmetry is supported by these bulk-sensitive experiments.

In order to make a clear distinction between the *d*-wave and extended *s*-wave gap symmetries, it is essential to determine precisely the superconducting gap along the diagonal direction (45° from the Cu-O bonding direction). If the diagonal gap is substantial, the *d*-wave gap symmetry can be ruled out, and only the extended *s*-wave gap symmetry is plausible. Several angle resolved photoemission spectroscopy (ARPES) experiments attempting to determine the magnitude of the diagonal gap (Δ_D) have led to contradictory conclusions. From the midpoint shift of the leading edges of the normal and superconducting ARPES data obtained with a 30 meV energy resolution, Shen *et al.*[11] found $\Delta_D\simeq0$ for an overdoped $Bi_2Sr_2CaCu_2O_{8+y}$ (BSCCO) with $T_c=78$ K and $\Delta_D=2-12$ meV for a nearly optimally doped BSCCO with $T_c=86$ K. By using the same criterion they estimated[11] the antinodal gap Δ_M to be about 12 meV, which is a factor of 2.8 smaller than the maximum gap (34 meV) deduced from scanning tunnelling spectroscopy for an overdoped BSCCO with $T_c=74.3$ K.[12] Using a fitting procedure for the ARPES spectra obtained with a 19 meV energy resolution, Ding *et al.* showed $\Delta_D=3.5\pm2.5$ meV (Ref. 13) or $\Delta_D=0\pm3$ meV (Ref. 14) in a BSCCO with $T_c=87$ K. With a better energy resolution (about 10 meV), Vobornik *et al.* found $\Delta_D=9\pm2$ meV for a heavily overdoped BSCCO with $T_c=60$ K.[15] On the other hand, from the midpoint shift of the leading edges of the spectra obtained with a 13–15 meV energy resolution, Gatt *et al.* found $\Delta_D=0$ in an overdoped BSCCO with $T_c=65$ K.[16] These contradictory conclusions about the magnitude of Δ_D may arise from a limited energy resolution and subjective criteria for extracting the gap. Therefore, the *d*-wave gap symmetry has not been firmly established for high-temperature superconductors.

Here we report high-resolution spectra of the second derivative $-d^2(\mathrm{Re}\,\Sigma)/d\omega^2$ of the real part of electron self-energy Σ along the diagonal ($\Gamma-Y$) direction (where $\omega=E_F-E-\Delta_D$) for a nonsuperconducting $La_{1.97}Sr_{0.03}CuO_4$ (LSCO) crystal and a superconducting $Bi_2Sr_2CaCu_2O_{8+y}$ crystal with $T_c=91$ K. The $-d^2(\mathrm{Re}\,\Sigma)/d\omega^2$ spectrum of the nonsuperconducting LSCO shows clear peak features, which match precisely with those in the phonon density of states obtained from neutron scattering. Similarly, if we assign $\Delta_D=7\pm1$ meV for the superconducting BSCCO, the peak features in $-d^2(\mathrm{Re}\,\Sigma)/d\omega^2$ of this compound also match precisely with those in the phonon density of states and the

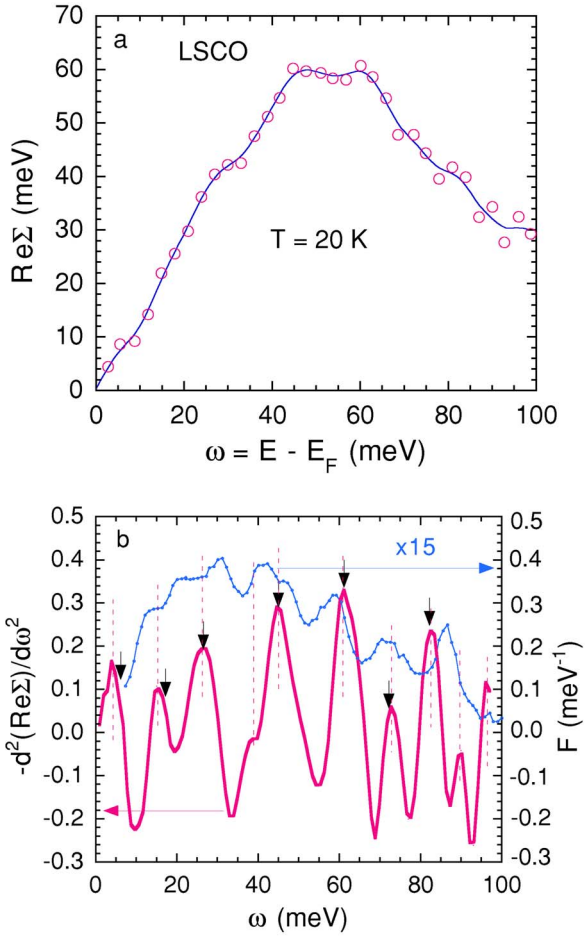

FIG. 1. (Color online) (a) The real part of the electron self-energy at 20 K for a nonsuperconducting $La_{1.97}Sr_{0.03}CuO_4$ crystal. The data are reproduced from Fig. 2 of Ref. 17. The solid line is a smoothed curve with a smoothing parameter $\Lambda=-2.5$ (see text). (b) $-d^2(\mathrm{Re}\,\Sigma)/d\omega^2$ spectrum (left scale) obtained from the smoothed curve in (a) and the phonon density of states (right scale) of $La_{1.85}Sr_{0.15}CuO_4$ at 20 K (Ref. 18). Downward arrows mark the positions of the boson modes in the electron-boson spectral function obtained using a maximum entropy method (Ref. 17) and vertical dashed lines indicate the positions of the peaks in $-d^2(\mathrm{Re}\,\Sigma)/d\omega^2$.

tunneling spectrum, and with the peak features in the normal-state $-d^2(\mathrm{Re}\,\Sigma)/d\omega^2$ spectra of several underdoped $La_{2-x}Sr_xCuO_4$ crystals. The present results rule out seemingly well accepted *d*-wave gap symmetry and strongly support an extended *s*-wave gap symmetry with eight line nodes.

In Fig. 1(a) we plot the real part of the electron self-energy at 20 K for a nonsuperconducting $La_{1.97}Sr_{0.03}CuO_4$ crystal. The data are reproduced from Fig. 2 of Ref. 17. The electron self-energy data are obtained from an ARPES spectrum, which is taken with an energy resolution of about 20 meV.[17] It is apparent that the electron self-energy shows fine structures associated with the bosonic modes coupled to electrons. In order to precisely determine the energies of the bosons, it is essential to take the second derivative of $\mathrm{Re}\,\Sigma$. Before taking the second derivative of $\mathrm{Re}\,\Sigma$, we need to obtain a smoothed curve for the data. We use a cubic spline interpolation method to smooth the data, which ensures no discontinuity in the first and second derivative. The smoothness of the interpolation is determined by a parameter Λ. The larger the Λ is, the smoother the curve is. The solid line in Fig. 1(a) is a smoothed curve with $\Lambda=-2.5$.

Figure 1(b) shows the $-d^2(\mathrm{Re}\,\Sigma)/d\omega^2$ spectrum obtained from the smoothed curve in Fig. 1(a). There are ten peak features at 4.2, 15.2, 26.2, 38.8, 45.0, 60.8, 72.8, 82.5, 89.6, and 96.1 meV. The energies of the peak features match very well with the boson energies (marked by downward arrows) in the electron-boson spectral function obtained using a maximum entropy method.[17] Such excellent agreement indicates that the smoothed curve with $\Lambda=-2.5$ represents a realistic average of the data.

In order to show that these fine structures in $-d^2(\mathrm{Re}\,\Sigma)/d\omega^2$ are associated with strong electron-phonon coupling, we compare these fine structures with those in the phonon density of states. It is apparent that nearly all the fine structures match precisely with those in the phonon density of states. The double peaks at 82.5 and 89.6 meV in $-d^2(\mathrm{Re}\,\Sigma)/d\omega^2$ should match with the single broad peak at 86.0 meV in the phonon density of states. Since the low-energy fine structures in self-energy are more difficult to resolve than the high-energy ones because of the same thermal broadening $(4.4k_BT)$,[19] the single broad peaks at 26.2 and 45.0 meV in $-d^2(\mathrm{Re}\,\Sigma)/d\omega^2$ should match with the double peaks in the phonon density of states. The peak at about 4.2 meV is consistent with the specific heat data[20] of $La_{1.85}Sr_{0.15}CuO_4$, which reveal an Einstein mode at about 4.3 meV. Therefore, nearly all the peak features in $-d^2(\mathrm{Re}\,\Sigma)/d\omega^2$ precisely match with those in the phonon density of states, which clearly indicates that the fine structures in $-d^2(\mathrm{Re}\,\Sigma)/d\omega^2$ are indeed caused by strong electron-phonon coupling.

In Fig. 2(a), we show the real part of the electron self-energy at 70 K for a superconducting $Bi_2Sr_2CaCu_2O_{8+y}$ crystal with $T_c=91$ K. The data are reproduced from Ref. 21. The electron self-energy data are obtained from an ARPES spectrum, which is taken with an energy resolution of about 10 meV.[21] By analogy to the $\mathrm{Re}\,\Sigma$ data of $\mathrm{Be}(10\bar{1}0)$ obtained with the same energy resolution,[22] we speculate that the uncertainty of the $\mathrm{Re}\,\Sigma$ data of BSCCO should be about ±1 meV. It is apparent that the fine structures of electron-boson coupling also show up in the electron self-energy of BSCCO. The energy of the highest peak is 66.0 meV, which is comparable with the energies (64–67 meV) of the kink features in the band dispersion curves of several overdoped BSCCO crystals.[23] The solid line is a smooth curve obtained using the cubic spline interpolation with $\Lambda=-4$. Because the energy resolution for the BSCCO data is two times better than that for the LSCO data, it is reasonable to choose $\Lambda=-4$ and -2.5 to smooth the BSCCO and LSCO data, respectively.

Taking the second derivative of the smoothed curve yields a $-d^2(\mathrm{Re}\,\Sigma)/d\omega^2$ spectrum, which is shown in Fig. 2(b). Here we have assigned $\omega=E_F-E-\Delta_D$ with $\Delta_D=7$ meV. There are six pronounced peak features at 5.8, 21.4, 38.3, 44.4, 60.0, and 76.2 meV, which are marked by vertical dashed lines. It is remarkable that the peak positions at 44.4, 60.0, and 76.2 meV for BSCCO match precisely with the

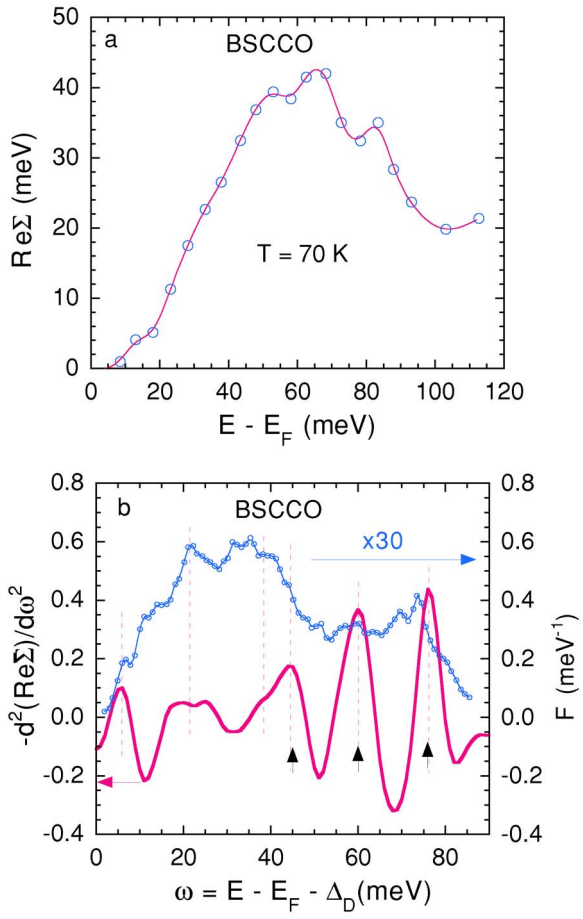

FIG. 2. (Color online) (a) The real part of the electron self-energy at 70 K for a superconducting BSCCO crystal with T_c =91 K. The data are reproduced from Ref. 21. The solid line is a smooth curve obtained using the cubic spline interpolation with Λ =−4. (b) The $-d^2(\mathrm{Re}\,\Sigma)/d\omega^2$ spectrum of a superconducting BSCCO crystal (left scale) and the phonon density of states (right scale) of BSCCO (Ref. 24). Here we have assigned $\omega=E_F-E-\Delta_D$ with Δ_D=7 meV. Upward arrows mark the positions of the peaks in the normal-state $-d^2(\mathrm{Re}\,\Sigma)/d\omega^2$ spectra in underdoped superconducting LSCO crystals (Ref. 17) and vertical dashed lines indicate the positions of the peaks in the $-d^2(\mathrm{Re}\,\Sigma)/d\omega^2$ spectrum of BSCCO.

peak positions (marked by upward arrows) at 45, 60, and 76 meV, which are consistently seen in the normal-state $-d^2(\mathrm{Re}\,\Sigma)/d\omega^2$ spectra of underdoped superconducting LSCO crystals.[17] The peak at 38.3 meV for BSCCO also lines up with the peak at 38.8 meV for $La_{1.97}Sr_{0.03}CuO_4$. Such excellent agreement indicates that the structures at 38.3, 44.4, 60.0, and 76.2 meV are caused by strong coupling to the CuO_2-plane related phonon modes and that the diagonal gap for BSCCO is 7±1 meV at 70 K.

In order to further show that the structures in $-d^2(\mathrm{Re}\,\Sigma)/d\omega^2$ are indeed associated with strong electron-phonon coupling, we compare these structures with those in the phonon density of states. It is striking that the peak features in the $-d^2(\mathrm{Re}\,\Sigma)/d\omega^2$ spectrum of $Bi_2Sr_2CaCu_2O_{8+y}$ match well with those in the phonon density of states obtained with neutron scattering.

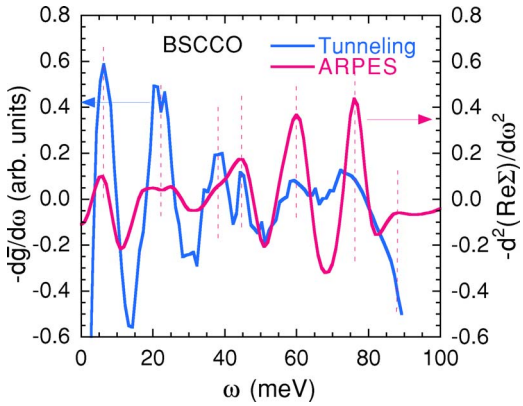

FIG. 3. (Color online) The $-d^2(\mathrm{Re}\,\Sigma)/d\omega^2$ spectrum and the $-d\bar{g}/d\omega$ tunneling spectrum of the BSCCO crystal (Ref. 25). The $-d\bar{g}/d\omega$ tunneling spectrum is reproduced from Ref. 25. Vertical dashed lines mark the peak positions in the $-d^2(\mathrm{Re}\,\Sigma)/d\omega^2$ spectrum.

In Fig. 3, we compare the $-d^2(\mathrm{Re}\,\Sigma)/d\omega^2$ spectrum with the $-d\bar{g}/d\omega$ tunneling spectrum.[25] Here $\bar{g}$ is the renormalized tunneling conductance.[25] One can clearly see that all the peak structures in $-d^2(\mathrm{Re}\,\Sigma)/d\omega^2$ of BSCCO line up precisely with those in the tunneling spectrum. Such quantitative agreement cannot be caused by any artifacts and must indicate that the fine structures in both $-d^2(\mathrm{Re}\,\Sigma)/d\omega^2$ and $-d\bar{g}/d\omega$ are due to strong electron-phonon coupling.

The substantial nonzero diagonal gap observed in the nearly optimally doped BSCCO rules out *d*-wave gap symmetry and strongly supports an extended *s*-wave gap symmetry with eight line nodes. The extended *s*-wave gap symmetry is also consistent with many other independent experiments.[26,27] These include phase-sensitive experiments based on out-of-plane Josephson tunneling,[28–30] single-particle tunneling spectroscopy,[31] Raman spectroscopy of heavily overdoped cuprates,[32] and nonlinear Meissner effect.[33] Moreover, the measurements of the physical properties that are related to low-energy quasiparticle excitations[7–10] are in quantitative agreement with an extended *s*-wave gap symmetry with eight line nodes.[26]

Now we discuss the validity of the above analyses. The basic assumption of the analyses is that the normal-state spectra display peak features at the characteristic phonon energies, and that the superconducting-state spectra exhibit peak features at the same energies shifted by the magnitude of the gap Δ_D along the diagonal direction. Our assumption for the superconducting state is not justified for a superconductor with a strongly anisotropic superconducting gap if the coupling to the large-momentum phonon modes dominates. On the other hand, if the coupling to large-momentum phonons is dominant, as in the case of conventional superconductors, the superconducting gap must be isotropic since exchange of phonons with large momenta effectively connects all points of the Fermi surface. In order to obtain a strongly anisotropic superconducting gap within strong electron-phonon coupling, the coupling to small momentum phonons must be dominant.[34] This is indeed the case for the ionic-crystal-like cuprate superconductors where the Coulomb screening is weak.[34] Then, the initial and scattered

electronic states connected by small momenta of phonons are close to each other so that the strong electron-phonon coupling features in the superconducting-state self-energy will be shifted by an angle-dependent gap. This is especially true for the spectra along the diagonal and antinodal directions where the superconducting density of states at Δ_D and Δ_M is singular in the case of the extended *s*-wave gap. This is because the singular superconducting density of states at the diagonal gap makes the weight of the zero-momentum phonon scattering (connecting the initial diagonal to the scattered diagonal electronic states) dominate.

In summary, we have analyzed the data of electron self-energy along the diagonal direction of a nonsuperconducting $La_{1.97}Sr_{0.03}CuO_4$ crystal and a superconducting $Bi_2Sr_2CaCu_2O_{8+y}$ crystal with $T_c=91$ K. Our analyses clearly show that the diagonal superconducting gap at 70 K is 7 ± 1 meV for the optimally doped BSCCO. The results rule out seemingly well accepted *d*-wave gap symmetry and strongly support an extended *s*-wave gap symmetry with eight line nodes. The present work places an essential constraint on the microscopic pairing mechanism of high-temperature superconductivity.

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