Lawrence Berkeley National Laboratory

Title

Electron-Phonon Coupling in High-Temperature Cuprate Superconductors as Revealed by Angle-resolved Photoemisson Spectroscopy

Permalink

https://escholarship.org/uc/item/5nd7x1dk

Authors

Zhou, X.J.
Hussain, Z.
Shen, Z.-X.

Publication Date

2005-05-01

Electron-Phonon Coupling in High-Temperature Cuprate Superconductors as Revealed by Angle-Resolved Photoemission Spectroscopy

X. J. Zhou [1,2,3], Z. Hussain[2], and Z.-X. Shen[1]

[1]Departments of Physics and Applied Physics, and Stanford Synchrotron Radiation Laboratory, Stanford University, Stanford, CA 94305, USA
[2]Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA
[3]National Laboratory for Superconductivity, Institute of Physics, Chinese Academy of Sciences, Beijing 100080, China

Cuprate oxide high-temperature superconductors are doped Mott insulators. The undoped parent compounds are antiferromagnetic insulators, and superconductivity occurs only when an appropriate number of charge carriers (electrons or holes) is introduced by doping. All cuprate materials contain CuO_2 planes (Figure 1a) in their crystal structure; the doped carriers are believed to go into these CuO_2 planes which are responsible for high temperature superconductivity. High temperature superconductors are characterized by their unusual physical properties, both in the superconducting state (below the superconducting transition temperature T_c) and in the normal state (above T_c). Since the discovery of high-temperature superconductivity in 1986 [1], these unusual physical properties and the mechanism of superconductivity have been prominent issues in condensed matter physics [2].

Angle-resolved photoemission spectroscopy (ARPES) is a powerful technique for studying the electronic structure of materials [3]. It has provided key insights in understanding high-temperature superconductors, such as determination of the Fermi surface, identification of an anisotropic superconducting gap, and observation of a pseudogap above T_c in underdoped samples. Several lengthy reviews of this subject already exist [4,5,6]. Recently, the dramatic improvement in the energy and momentum resolution of ARPES has led to a series of new discoveries not thought possible only a decade ago. In this technical report, we highlight some of the latest developments in this technique by focusing on experiments on many-body effects in high-T_c materials carried out at the Stanford Synchrotron Radiation Laboratory and at the Advanced Light Source.

The many-body effect refers to interactions of electrons with other entities, such as other electrons, disorder or impurities, or collective excitations like phonons, magnons, and so on. These interactions give rise to a change of the electron dynamics, which is described by the electron self-energy $\Sigma = \mathrm{Re}\,\Sigma + i\,\mathrm{Im}\,\Sigma$. ARPES can measure these quantities directly because, in the sudden approximation, it measures the single-particle spectral function $A(k,\omega)$, where

$$A(k,\omega) = \frac{1}{\pi} \frac{|\mathrm{Im}\,\Sigma|}{[\hbar\omega - \varepsilon_k - \mathrm{Re}\,\Sigma]^2 + [\mathrm{Im}\,\Sigma]^2} \,. \tag{1}$$

The real part of the self-energy, $\mathrm{Re}\,\Sigma$, is related to the renormalization of the quasiparticle dispersion (energy as a function of momentum); the imaginary part of the self-energy,

Im Σ, is related to the quasiparticle scattering rate (or lifetime); and ε_k represents the bare-band dispersion in the absence of these interactions.

Advances in the ARPES technique, particularly the advent of the ability to collect data simultaneously over multiple angles with a modern electron energy analyzer, has provided a convenient way of extracting the electron self-energy, as exemplified in Figure 2. The raw data (Figure 2a) is a two-dimensional image representing photoelectron intensity (false color scale) as a function of electron energy and emission angle (and hence momentum). The traditional way to visualize the photoemission data is by means of so-called energy distribution curves (EDCs), which represent photoelectron intensity as a function of energy for a given momentum. The 2D image comprising the raw data is then equivalent to a number of EDCs at different momenta (Figure 2b). However, the EDC lineshape is usually complicated by a background and the Fermi function cutoff, which makes it difficult to extract the electron self-energy precisely.

A new way to visualize the 2D data is to analyze photoelectron intensity as a function of momentum for a given electron kinetic energy [7] by means of momentum distribution curves (MDCs) [8]. This approach provides a different way of extracting the electron self-energy. As shown in Figure 2c, the MDCs exhibit well-defined peaks with flat backgrounds; moreover, they can be fitted by a Lorentzian lineshape. When the bandwidth is large, the band dispersion ε_k can be approximated as $\varepsilon_k = v_0 k$ in the vicinity of the Fermi level. Under the condition that the electron self-energy shows weak momentum dependence, $A(k,\omega)$ indeed exhibits a Lorentzian lineshape as a function of k for a given binding energy $\hbar\omega$. By fitting a series of MDCs at different binding energies to obtain the MDC position $\overset{?}{k}$ and width Γ (full-width at half maximum, FWHM), one obtains the energy-momentum dispersion relation and the variation of MDC as a function of energy (Figure 2d) [9]. From these, one can further extract electron self-energy directly as: $\mathrm{Re}\,\Sigma = \hbar\omega - \overset{?}{k}v_o$ and $\mathrm{Im}\,\Sigma = \Gamma v_o/2$.

We now proceed to briefly discuss three aspects of progress in probing many-body effects in high-T_c materials: (1) Electron-phonon coupling along the $(0,0)$–(π,π) nodal direction; (2) Electron-phonon coupling near the $(\pi,0)$ antinodal region; and (3) the possibility of identification of fine structure in the electron self-energy.

1. Electron-phonon coupling along the (0,0)–(π,π) nodal direction

The nodal direction denotes the $(0,0)$–(π,π) direction in the Brillouin zone (Figure 1b). The *d*-wave superconducting gap is zero along this particular direction. As shown in Figure 3 and Figure 4a, the energy-momentum dispersion curve exhibits an abrupt slope change ("kink") near 70 meV. The kink is accompanied by an accelerated drop in the MDC width at a similar energy scale (Figure 4b). The existence of the kink has been well established as ubiquitous in hole-doped cuprate materials [8,10-16]:

1. It is present in various hole-doped cuprate materials, including $Bi_2Sr_2CaCu_2O_8$ (Bi2212), $Bi_2Sr_2CuO_6$ (Bi2201), $(La_{2-x}Sr_x)CuO_4$ (LSCO) and others. The energy scale (in the range of 50–70 meV) at which the kink occurs is similar for the various systems.
2. It is present both below T_c and above T_c.
3. It is present over an entire doping range (Figure 4a). The kink effect is stronger in the underdoped region and gets weaker with increasing doping.

While there is a consensus on the data, the exact meaning of the data is still under discussion. The first issue concerns whether the kink in the normal state is related to an energy scale. Valla et al. argued that the system is quantum critical and thus has no energy scale, even though a band renormalization is present in the data [8]. Since their data do not show a sudden change in the scattering rate at the corresponding energy, they attributed the kink in Bi2212 above T_c to the marginal Fermi liquid (MFL) behavior without an energy scale [13]. Others believe the existence of energy scale in the normal and superconducting states has a common origin, i.e., coupling of quasiparticles with low-energy collective excitations (bosons) [10-12]. The sharp kink structure in dispersion and concomitant existence of a drop in the scattering rate which is becoming increasingly clear with the improvement of signal to noise in the data, as exemplified in underdoped LSCO (x=0.063) in the normal state (Figure 4b) [9], are apparently hard to reconcile with the MFL behavior.

A further issue concerns the origin of the bosons involved in the coupling, with a magnetic resonance mode [12,13] and optical phonons [11] being possible candidates considered. The phonon interpretation is based on the fact that the sudden band renormalization (or "kink") effect is seen for different cuprate materials, at different temperatures, and at a similar energy scale over the entire doping range [11]. For the nodal kink, the phonon considered in the early work was the half-breathing mode, which shows an anomaly in neutron experiments [17,18]. Unlike the phonons, which are similar in all cuprates, the magnetic resonance (at correct energy) is observed only in certain materials and only below T_c. The absence of the magnetic mode in LSCO and the appearance of magnetic mode only below T_c in some cuprate materials are not consistent with its being the cause of the universal presence of the kink effect. Whether the magnetic resonance can cause any additional effect is still an active research topic [19,20].

To test the idea of electron-phonon coupling, an isotope exchange experiment has been carried out [16]. When exchanging ^{18}O and ^{16}O in Bi2212, a strong isotope effect has been reported in the nodal dispersions (Figure 5). Surprisingly, however, the isotope effect mainly appears in the high binding energy region above the kink energy; at the lower binding energy near the Fermi level, the effect is minimal. This is quite different from the conventional electron-phonon coupling where isotope substitution will result in a small shift of phonon energy while keeping most of the dispersion intact. The origin of this behavior is still being investigated.

It is interesting to note in Figure 4a that the energy scale of the kink also serves as a dividing point where the high energy and lower energy dispersions display different doping dependence. While the high energy part of the dispersion varies strongly with doping, the dispersion converges below about 50 meV, revealing a behaviour that is nearly independent of doping. The common behaviour below 50 meV is quantified using the corresponding quasiparticle velocity, $v=\delta\varepsilon/\delta k$, and the low-energy Fermi velocity, v_F, is nearly a constant for many different cuprate materials [15]. This universality in nodal Fermi velocity is most striking for the LSCO family, where data cover the entire doping range (x) over which the physical properties vary from insulator ($0 \leq x < 0.03$), to superconductors ($0.05 < x < 0.25$) and to overdoped non-superconducting metal ($x > 0.25$).

2. Electron-phonon coupling near the (π,0) antinodal region

The antinodal region refers to the (π,0) region in the Brillouin zone where the *d*-wave superconducting gap has a maximum (Figure 1b). It has been shown that the antinodal region exhibits different behaviors from the nodal region, particularly in the underdoped samples [21,9]. Recently, a low-energy kink was also identified near the (π,0) antinodal region in Bi2212 [12,22-24]. This observation was made possible thanks to the clear resolution of the bi-layer splitting [25]. As there are two adjacent CuO_2 planes in a unit cell of Bi2212, these give rise to two Fermi surface sheets from the higher-binding-energy bonding band (B) (thick red curves in Figure 6c) and the lower-binding- energy antibonding band (A) (thick black curves in Figure 6c).

Consider a cut along (π,π)–(-π,π) across (π,0) in Bi2212, both above T_c (Figure 6a) and below T_c (Figure 6b) [22]. Superimposed are the dispersion of the bonding band determined from the MDC (red lines) and antibonding band from the EDC (black dots). When the bandwidth is narrow, the applicability of the MDC method in obtaining dispersion becomes questionable so one has to resort to the traditional EDC method. In the normal state, the bonding-band dispersion (Figure 6a) is nearly linear and featureless in the energy range of interest. Upon cooling to 10 K (Figure 6b), the dispersion, as well as the near-E_F spectral weight, is radically changed. In addition to the opening of a superconducting gap, there is a clear kink in the dispersion around 40 meV.

Gromko et al.[22] reported that the antinodal kink effect appears only in the superconducting state and gets stronger with decreasing temperature. Their momentum-dependence measurements show that the kink effect is strong near (π,0) and weakens dramatically when the momentum moves away from the (π,0) point. Excluding the possibility that this is a by-product of a superconducting-gap opening, they attributed the antinodal kink to the coupling of electrons to a bosonic excitation, such as a phonon or a collective magnetic excitation. The prime candidate they considered is the magnetic-resonance mode observed in inelastic neutron scattering experiments.

An alternative interpretation of the antinodal kink was proposed by Cuk et al. [24]. On a general ground, the antinodal kink can be observed in deeply overdoped Bi2212, but no evidence of a spin resonance exists at this doping level. Specifically, the key observation that prompted them to question the spin-resonance interpretation is the unraveling of the existence of the antinodal kink even in the normal state. This observation was made possible by utilizing the EDC method and high-quality data with very good signal-to-noise ratio. The MDC method is not appropriate when the assumed linear approximation of the bare band fails near (π,0), where the band bottom is close to the Fermi level E_F. Figures 7(a1), 7(b1), and 7(c) show dispersions in the normal state that reveal an approximately 40 meV energy scale that has eluded detection previously. This coupling is also found to be more extended in the Brillouin zone than previously reported [24].

Based on these new observations, and coupled with theoretical simulations, Cuk and Devereaux et al. proposed the coupling of the B_{1g} phonons as the origin of the antinodal kink in Bi2212 [24,26]. This phonon mode represents out-of-plane, out-of-phase vibration of oxygen in the CuO_2 planes with a frequency around 36 meV in Bi2212. Applying simple symmetry considerations and kinematic constraints, it is found that this B_{1g} buckling mode involves small momentum transfers and couples strongly to electronic states near the antinode [26]. Band renormalization effects are also found to be strongest

in the superconducting state near the antinode, in full agreement with ARPES data (Figure 8). The dramatic temperature dependence stems from a substantial change in the electronic occupation distribution and the opening of the superconducting gap [24,26]. In contrast, the in-plane Cu-O breathing modes involve large momentum transfers and couple strongly to nodal electronic states (Figure 8) [26].

3. Identification of fine structure in the electron self-energy

For conventional superconductors, the successful extraction of the phonon spectral function, or the Eliashberg function, $\alpha^2 F(\omega)$, from electron tunneling data played a decisive role in cementing the consensus on a phonon-mediated mechanism of superconductivity. For high-temperature superconductors, the extraction of the bosonic spectral function will at first provide fingerprints for more definitive identification of the nature of the bosons involved in the coupling. It will also provide key information on the nature of superconductivity pairing.

With the availability of high-resolution data for the electron self-energy, in principle it is possible to extract the electron-boson coupling information quantitatively. For a conventional metal, it is well-known that the real part of the self-energy ReΣ is related to the Eliashberg function $\alpha^2 F(\omega)$ by:

$$\mathrm{Re}\,\Sigma = \int_0^\infty d\omega \alpha^2 F(\omega) G\left(\frac{\varepsilon}{kT}, \frac{\omega}{kT}\right), \text{ where} \tag{2}$$

$$G(y,y') = \int_{-\infty}^\infty dx \frac{2y'}{x^2 - y'^2} f(x+y)$$

with *f(x)* being the Fermi-Dirac function. Unfortunately, since noise in the data is inevitable, this inversion problem is ill-posed mathematically. Very recently, Shi et al. have made an important advance in extracting the Eliashberg function from ARPES data by means of the maximum entropy method (MEM) and successfully applied the method to Be surface states [27,28].

Initial efforts have been made to extend this approach to underdoped LSCO and evidence for electron coupling to several phonon modes has been uncovered [29]. We note that, in order to be able to identify fine structure in the electron self-energy, it is imperative to have both a high resolution and data with good statistics. These requirements have made the experiment highly challenging because of the necessity to compromise between two conflicting requirements for a synchrotron light source: high energy resolution and high photon flux. Further improvements in photoemission experiments will likely enable a detailed understanding of the boson modes coupled to electrons, and provide critical information for the pairing mechanism.

References
1. J. G. Bednorz and K. A. Muller, *Z. Phys. B* **64**, 189 (1986).
2. See, e.g., reviews in the special issue on correlated electron systems, *Science* **288**, 461 (2000).
3. S. Hüfner, *Photoelectron Spectroscopy: Principles and Applications*, (Springer, Berlin, 1995).
4. Z.-X. Shen and D. S. Dessau, *Phys. Rep.* **253**, 1(1995).
5 . A. Damascelli, Z. Hussain and Z.-X. Shen, *Rev. Mod. Phys.* **75**, 473 (2003).
6. J. C. Campuzano, M. R. Norma and M. Randeria, in *Physics of Superconductors*, Vol. II, ed. K. H. Bennemann and J. B. Ketterson (Springer, Berlin, 2004), pp. 167-273.
7. P. Aebi et al., *Phys. Rev. Lett.* **72**, 2757 (1994).
8. T. Valla et al., *Science* **285**, 2110(1999).
9. X. J. Zhou et al., *Phys. Rev. Lett.* **92**, 187001 (2004).
10. P. V. Bogdanov et al., *Phys. Rev. Lett.* **85**, 2581 (2000).
11. A. Lanzara et al., *Nature* **412**, 510 (2001).
12. A. Kaminski et al., *Phys. Rev. Lett.* **86**, 1070 (2001).
13. P. D. Johnson et al., *Phys. Rev. Lett.* **87**, 177007(2001).
14. S. V. Borisenko et al., *Phys. Rev. Lett.* **90**, 207001 (2003).
15. X. J. Zhou et al., *Nature* **423**, 398 (2003).
16. G.-H. Gweon et al., *Nature* **430**, 187 (2004).
17. L. Pintschovius and M. Braden, *Phys. Rev. B* **60**, R15039 (1999).
18. R. J. McQueeney et al., *Phys. Rev. Lett.* **82**, 628 (1999).
19. H.-Y. Kee, S. Kivelson and G. Aeppli, *Phys. Rev. Lett.* **88**, 257002 (2002).
20. Ar. Abanov et al., *Phys. Rev. Lett.* **89**, 17702 (2002).
21. Z.-X. Shen and J. R. Schrieffer, *Phys. Rev. Lett.* **78**, 1771 (1997).
22. A. D. Gromko et al., *Phys. Rev. B* **68**, 174520 (2003).
23. T. K. Kim et al., *Phys. Rev. Lett.* **91**, 167002 (2003).
24. T. Cuk et al., *Phys. Rev. Lett.* **93**, 117003 (2004).
25. D. L. Feng et al., *Phys. Rev. Lett.* **86**, 5550 (2001); Y. D. Chuang et al., *Phys. Rev. Lett.* **87**, 117002 (2001); P. V. Bogdanov et al., *Phys. Rev. B* **64**, 180505 (2001).
26. T. P. Devereaux et al., *Phys. Rev. Lett.* **93**, 117004(2004).
27. J. R. Shi et al., *Phys. Rev. Lett.* **92**, 186401(2004).
28. S.-J. Tang et al., *physica status solidi* (*b)* **241**, 2345 (2004).
29. X. J. Zhou et al., cond-mat/0405130, submitted to *Phys. Rev. Lett.*

Figure captions:

Figure 1. (a) Schematic of the real-space CuO_2 plane. The CuO_2 plane consists of copper (pink solid circles) and oxygen (black open circles). (b) The corresponding Brillouin zone in a reciprocal space. In the first Brillouin zone, the area near $(\pi/2,\pi/2)$ (denoted as red circle) is referred to as nodal region, and the $(0,0)$–(π,π) direction is the nodal direction (red arrow). The area near $(\pi,0)$ and $(0,\pi)$ is referred to as the antinodal region (shaded circles). The blue solid line shows a schematic Fermi surface.

Figure 2. Illustration of the MDC method for extracting the electron self-energy [9]. (a) Raw photoemission data for LSCO with x=0.063 ($T_c \approx 12K$) along the (0,0)–(π,π) nodal direction at 20 K. The two-dimensional data represent the photoelectron intensity (denoted by false color) as a function of energy and momentum. (b) Energy distribution curves (EDCs) at different momenta. The EDC colored red corresponds to the Fermi momentum k_F. (c) Momentum distribution curves (MDCs) at different binding energies. The MDC colored red corresponds to the Fermi level. (d) Energy–momentum dispersion relation extracted by the MDC method. The inset shows the MDC width as a function of energy.

Figure 3. Ubiquitous existence of a kink in the nodal dispersion of various cuprate materials [11]. Top panels (a, b, c) plot dispersions along (0, 0)–(π,π) direction (except for panel b inset, which is off this direction) as a function of the rescaled momentum k' for different samples and at different doping levels (δ): (a) LSCO at 20 K, (b) Bi2212 in superconducting state at 20 K, and (c) Bi2201 in normal state at 30 K. Dotted lines are guides to the eye. Inset in (b) shows that the kinks in the dispersions off the (0, 0)–(π,π) direction sharpen upon moving away from the nodal direction. The black arrows indicate the position of the kink in the dispersions. Panels (d) and (e) show the temperature dependence of the dispersions for (d) optimally doped LSCO (x=0.15) and (e) optimally-doped Bi2221, respectively. Panel (f) shows the doping dependence of the effective electron-phonon coupling strength λ' along the (0, 0)–(π,π) direction. Data are shown for LSCO (filled triangles), Nd-doped LSCO (1/8 doping; filled diamonds), Bi2201 (filled squares), and Bi2212 (filled circles in the first Brillouin zone and unfilled circles in the second zone). The different shadings represent data obtained in different experimental runs. Shaded area is a guide to the eye.

Figure 4. Doping dependence of the nodal electron dynamics in LSCO and universal nodal Fermi velocity [15]. (a) Dispersion of LSCO with various doping levels (x $\approx$ 0.03 to 0.30) measured at 20 K along the (0,0)–(π,π) nodal direction. The arrow indicates the position of kink that separates the dispersion into high-energy and low-energy parts with different slopes. (b). Scattering rate as measured by MDC width (full-width-at-half-maximum, FWHM) of the LSCO (x = 0.063) sample measured at 20 K. The arrow indicates a drop at an energy $\approx$ 70 meV.

Figure 5. Isotope-induced changes of the nodal dispersion [16]. The data were taken on optimally doped $Bi_2Sr_2CaCu_2O_8$ samples ($T_c \approx$ 91 to 92 K) with different oxygen isotopes [16]O and [18]O at T $\approx$ 25 K along the nodal direction. The low energy dispersion is nearly isotope-independent, while the high energy dispersion is isotope-dependent. The effect is reversible by isotope re-substitution (green). Inset shows the real part of the electron self-energy, ReΣ, obtained from the dispersion by subtracting a line approximation for the one-electron band ε_k, connecting two points (one at E_F and the other at a 300-meV binding energy) of the [18]O dispersion.

Figure 6. Antinodal kink near (π,0) in a heavily overdoped Bi2212 sample ($T_c \approx$ 58 K) [22]. (a) Normal-state data (T=85 K) near the antinodal region. (b) Superconducting-state

data from the same sample at 10 K, showing the emergence of a dispersion kink in the bilayer split-B band. The B band dispersions (red curves) were determined by fitting MDC peak positions. The black dots represent A band EDC peak positions. (c) Brillouin zone with bonding band B (thick red) and antibonding band A (thick black) Fermi surfaces, as well as momentum-cut locations for panels (a) and (b) (blue bars).

Figure 7. Antinodal kink near $(\pi,0)$ in the normal state (a1,b1,c) and superconducting state (a2,b2) in an optimally-doped Bi2212 [24]. The dispersions in a1, b1, and c were derived by the EDC method; the position of the momentum cuts is labeled in the insets. The red dots are the data; the fit to the curve (black dashed line) below the 40-meV line is a guide to the eye. The dispersions at the same location in the superconducting state (10 K) are shown in (a2) and (b2), which were derived by the MDC method (blue circles). Also plotted in (a2) and (b2) are the peak (blue squares, I) and hump positions (blue squares, II) of the EDCs for comparison. The inset of (a2) shows the expected behavior of a Bogoliubov-type gap opening. The s-like shape below the gap energy is an artifact of the way the MDC method handles the backbend of the Bogoliubov quasiparticle. (d). Kink positions as a function of momentum cuts in the antinodal region.

Figure 8. Comparison between the calculated and measured spectral function in Bi2212 including electron-phonon coupling for three different momentum cuts (a, b, c) through the Brillouin zone [26]. (a1,b1,c1) and (a2,b2,c2) show the calculated spectral functions in the normal and superconducting states, respectively. The measured spectral functions are shown in (a3,b3,c3) for the normal state and in (a4,b4,c4) for the superconducting state. The corresponding momentum cuts a, b, and c are shown in the rightmost panel. The red markers in the superconducting state indicate 70 meV. The simulation includes B_{1g} oxygen buckling mode and half-breathing mode.