

## Change of Fermi-surface topology in $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ with doping

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We report the observation of a change in Fermi-surface topology of  $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$  with doping. By collecting high-statistics angle-resolved photoemission spectroscopy data from moderately and highly overdoped samples and dividing the data by the Fermi function, we answer a long-standing question about the Fermi-surface shape of  $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$  close to the  $(\pi, 0)$  point. For moderately overdoped samples ( $T_c = 80$  K) we find that both the bonding and antibonding sheets of the Fermi surface are hole like, but for a doping level corresponding to  $T_c = 55$  K we find that the antibonding sheet becomes electron like. Similar observations of a topology change were observed in  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$  and in  $\text{Bi}_2\text{Sr}_2\text{CuO}_{6+\delta}$ . On the other hand, whereas this critical doping value in single-layer materials corresponds to a  $T_c$  near zero, it occurs at a smaller doping value in the double-layer case where  $T_c$  is still quite high (the difference in doping levels is due to the bilayer splitting). This argues against a van Hove singularity scenario for cuprate superconductivity.

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The Fermi surface is a fundamental property in condensed-matter physics. In recent years there has been a lively debate about the shape of the Fermi surface of one of the most frequently studied high-temperature superconductors:  $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ .<sup>1,2</sup> Initially, the Fermi surface of this compound was determined by angle-resolved photoemission spectroscopy (ARPES) to be hole like and consistent with Luttinger's theorem.<sup>3</sup> Later there were reports of an electron like Fermi surface when measurements were performed at higher photon energies.<sup>4,5</sup> High-momentum-resolution studies utilizing new-generation electron analyzers reestablished the hole like shape of the Fermi surface for optimal doping.<sup>6,7</sup> The observation of bilayer splitting in the overdoped regime<sup>8</sup> provided further evidence that at least the bonding sheet of the Fermi surface is hole like for a wide range of dopings. However, this study did not address the question of the shape of the antibonding sheet of the Fermi surface. For a long time, the answer to this question remained elusive, as the antibonding band near  $(\pi, 0)$  is located very close to the chemical potential. It is important to determine the exact shape of the whole Fermi surface, as it potentially affects transport and collective properties. Knowledge of the band dispersion in this region of the Brillouin zone is also of importance for theoretical studies of self-energy effects in ARPES and tunneling, modeling of optical conductivity, and calculations of the dynamic magnetic response. In a broader scope, it was previously shown that a change in the topology of the Fermi surface occurs in overdoped  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$  (LSCO) (Refs. 9 and 10) and heavily overdoped single-layer  $\text{Bi}_2\text{Sr}_2\text{CuO}_{6+\delta}$  (Ref. 11); therefore, this phenomenon should be a generic property of hole-doped cuprates. Here, we present high-resolution ARPES data measured to a high degree of statistical accuracy in order to determine the evolution of the Fermi surface with doping. We find that for moderately doped samples, both sheets of the Fermi surface are hole like, while at higher doping levels the antibonding band becomes electron like. This change is

not accompanied by any abrupt change in the critical temperature at this particular value of doping. The lack of correlation of the topology change with  $T_c$  argues against a van Hove singularity scenario for cuprate superconductivity.

The overdoped thin-film samples were grown using a magnetron sputtering technique on a  $\text{SrTiO}_3$  substrate.<sup>12</sup> They were mounted with  $\Gamma$ - $M$  parallel to the photon polarization and cleaved *in situ* at pressures of less than  $2 \times 10^{-11}$  Torr. Measurements were carried out at the Synchrotron Radiation Center in Madison, Wisconsin, on the U1 undulator beamline supplying  $10^{12}$  photons/sec, using a Scienta SES 50 electron analyzer with an energy resolution of 20 meV and momentum resolution of  $0.01 \text{ \AA}^{-1}$  for a photon energy of 22 eV. The value of the chemical potential was determined by measuring the Fermi edge of a gold film evaporated onto silicon in electrical and thermal contact with the sample. This value was stable to within 0.5 meV as verified by periodic measurements of the gold reference throughout the experiment.

One of the limitations of the ARPES technique is the fact that it only measures the occupied part of the spectrum. The Fermi cutoff makes it difficult to directly analyze the data close to the chemical potential. To combat these limitations, we have exploited a method of gaining information about the states close to and above the chemical potential, which relies on dividing the ARPES data by the resolution-broadened Fermi function.<sup>13-15</sup> This function is easily obtained by fitting the gold reference spectra with a Fermi function. We renormalize the fitted Fermi function, so that its maximum amplitude is equal to 1, and then divide by it the ARPES spectra for the sample. The result very well approximates the spectral function  $A(k, \omega)$  modulo matrix elements (which are almost constant within a small range of momenta). The effectiveness of this method depends on two conditions: the sample temperature and the statistics of the data. Working at high temperature increases the spectral weight above the chemical potential and thus allows us to extract the data

there with less noise. For low temperatures, data of high statistics are required, as the noise at energies above the chemical potential is rapidly amplified since the data are divided by the small values of the Fermi function. Given the high statistics of our data, we can reliably extract the spectral function for samples at  $T=100$  K up to energies of  $\sim 50$  meV above the chemical potential. Stability of the chemical potential is essential for successful application of this method. This was monitored frequently during the experiment, and the typical variation of its value was very small, of the order of 0.5 meV. We note that this is the dominant contribution to the error in our results; the errors arising from peak fitting procedures are smaller (for peaks near the chemical potential). We also note that the accuracy of fitting the peak position depends crucially on the statistics and its functional form and much less on the width of the peak. Another experimental consideration is the contribution to the measured electron intensity from the second-order light, which is always present in synchrotron beamlines. In the case of our beamline this contribution is very small (2%). We determine this contribution by looking at the average intensity far above the chemical potential and then subtracting it from the data before performing the division operation.

We illustrate the division by the Fermi function in Fig. 1. In panel (a) the raw ARPES data [measured in the form of energy distribution curves (EDC's)] for a cut parallel to the  $(\pi, -\pi)$ - $(\pi, \pi)$  direction are shown, and in panel (b) the result of the division of the Fermi function is plotted. In the raw data there are two clearly visible features: (i) dispersing peaks corresponding to the bonding band and (ii) “nondispersive” peaks near the chemical potential corresponding to the antibonding band. As stated above, it is difficult to determine the band position and dispersion of the antibonding band from such data. In contrast, it is quite easy to do so when the data are divided by the Fermi function, as shown in panel (b). Here the dispersion of both the bonding and antibonding bands is clearly visible at, and even above, the chemical potential. Such an approach allows us to determine the precise location of the bottom of both bands even in close proximity to the chemical potential. We next examine the accuracy of the above method. To do this we present a sample spectral function shown as a blue solid line in panel (c) of Fig. 1. We then multiply it by the Fermi function, convolve with a Gaussian to emulate the energy resolution-broadening, and then divide the result by the resolution-broadened Fermi function. The reconstructed spectral function (dashed red curve) compares quite well to the original spectral function. We then extract the peak dispersion from both curves and compare the results in panel (d) of Fig. 1. Both dispersions are in very good agreement—in the region of the chemical potential, the differences are within experimental error bars of 0.5 meV.

First, we examine the case of a moderately overdoped sample ( $T_c=80$  K). In Fig. 2 we plot the ARPES data divided by the Fermi function for a cut parallel to the  $(\pi, -\pi)$ - $(\pi, \pi)$  direction. The first panel shows the divided EDC curves in the proximity of the  $(\pi, 0)$  point, while in panel (b), we show the peak dispersions for both bonding and antibonding bands extracted from the EDC data by fitting them with a sum of

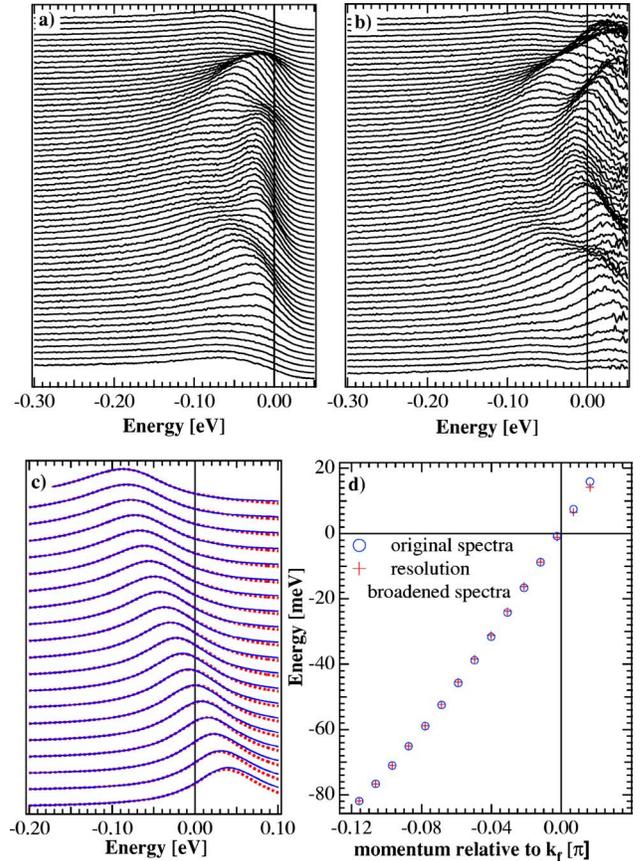


FIG. 1. (Color online) Illustration of the division by the Fermi function method at  $T=100$  K for an overdoped sample ( $T_c=55$  K) along the cut  $(0.8\pi, -0.3\pi)$ - $(0.8\pi, 0.3\pi)$ . (a) Raw ARPES data. (b) Data from (a) divided by the resolution-broadened Fermi function. (c) Effect of resolution broadening on extraction of the spectral function peaks: solid blue line is a model spectral function, red dashed line is the same spectral function after multiplying by the Fermi function, convolution with the experimental energy resolution function, and division by the resolution-broadened Fermi function. (d) Dispersion obtained from the peak positions of panel (c).

two Lorentzians. The deviations from the parabolic dispersion originate from the fact that the Lorentzian fitting procedure is less accurate for the bonding peak once it is far below the chemical potential and thus very broad. This does not affect our conclusions, since we are interested in the energy position of the bottom of the antibonding band, where this fitting procedure works very well. We note that the bottoms of both bands along this direction lie below the chemical potential, which means that for this doping value both sheets of the Fermi surface remain hole like. To quantify this we plot in panel (c) the EDC's at the  $(\pi, 0)$  and  $(0.9\pi, 0)$  points and fit them using a combination of two Lorentzian functions, corresponding to the bonding and antibonding peaks. The  $(\pi, 0)$  point is at  $-7$  meV and  $-102$  meV for the antibonding and bonding bands respectively.

Next, we turn to the most heavily overdoped sample ( $T_c=55$  K) that we could obtain. The data for this sample are shown in Fig. 3. In panels (a) and (b) we show the EDC's and extracted peak dispersion along the  $(0.9\pi, -0.3\pi)$ - $(0.9\pi, 0.3\pi)$  cut. As in the previous case, these data show

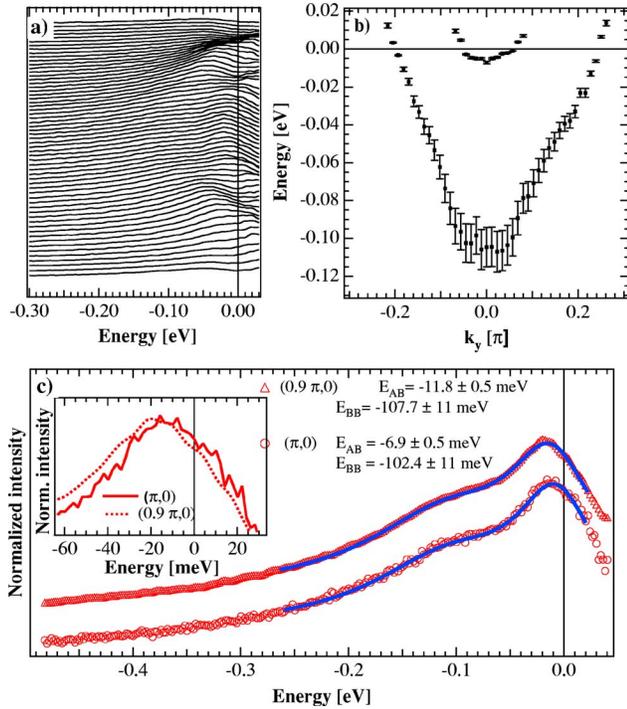


FIG. 2. (Color online) Data along the  $(\pi, -\pi)$  to  $(\pi, \pi)$  direction for a moderately overdoped sample of  $T_c=80$  K at  $T=100$  K. (a) EDC data divided by the Fermi function. (b) Dispersion extracted from a two-Lorentzian fit to the EDC's. (c) EDC at  $(\pi,0)$  and  $(0.9\pi,0)$  divided by the Fermi function (red circles and triangles) and a two-Lorentzian fit (blue lines).  $E_{AB}$  and  $E_{BB}$  are the positions of the antibonding and bonding peaks. Inset: magnified region close to the chemical potential.

that the bottoms of both bands lie below the chemical potential. However, the data obtained along the Brillouin zone boundary [i.e., along the  $(\pi, -0.3\pi)$ - $(\pi, 0.3\pi)$  cut], shown in panels (c) and (d), are different. Here, the bottom of the antibonding band is located slightly above the chemical potential. To check the exact location of the antibonding band we plot the EDC curves at  $(\pi,0)$  and  $(0.9\pi,0)$  in panel (e). Each EDC is fit with the sum of two Lorentzian functions to precisely determine the energy locations of the peaks. While the antibonding peak at  $(0.9\pi,0)$  is located at 2.5 meV below the chemical potential [consistent with the conclusions from data in panels (a) and (b)], the same peak at  $(\pi,0)$  lies at 2 meV above the chemical potential. This is clear evidence that the antibonding Fermi surface closes before reaching the zone boundary and therefore becomes electron like. The Fermi crossing along  $(0,0)$ - $(\pi,0)$  occurs close to  $(0.95\pi,0)$  based on linear interpolation.

The extraction of the Fermi-surface contours from the data using the standard method of plotting the intensity within a small energy range about the chemical potential over the whole Brillouin zone is quite difficult in this case. The main reasons for this are the presence of a background<sup>16</sup> and the relatively wide EDC peaks in the normal state combined with the close proximity to the chemical potential of the antibonding band at  $(\pi,0)$ . To better illustrate the topologies, in Fig. 4 we plot Fermi surfaces resulting from tight-

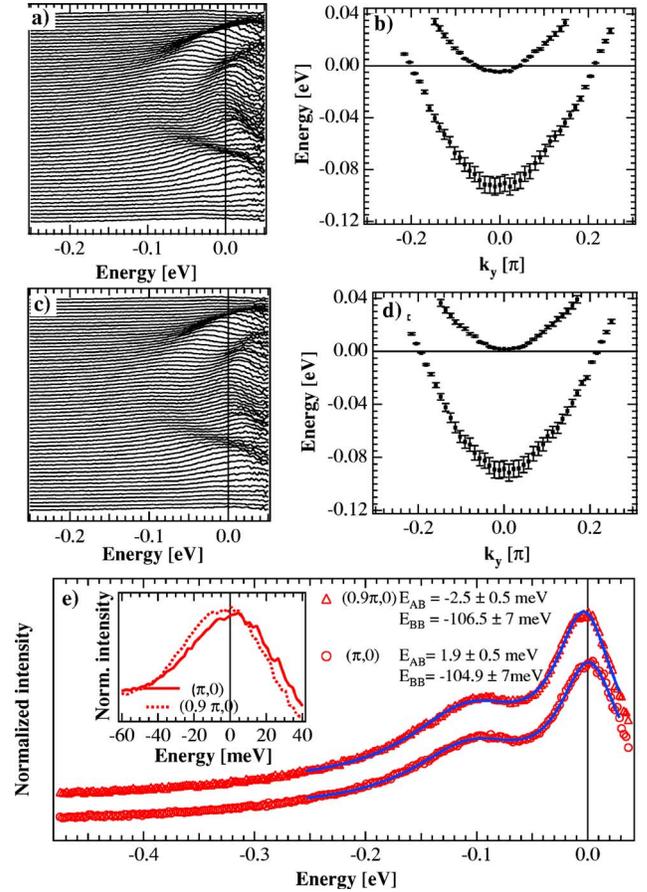


FIG. 3. (Color online) Data parallel to the  $(\pi, -\pi)$  to  $(\pi, \pi)$  direction for a heavily overdoped sample of  $T_c=55$  K at  $T=100$  K. (a) EDC data divided by the Fermi function along the  $(0.9\pi, -0.3\pi)$ - $(0.9\pi, 0.3\pi)$  cut. (b) Dispersion extracted from a two-Lorentzian fit to the EDC data shown in (a). (c) EDC data divided by the Fermi function for a  $(\pi, -0.3\pi)$ - $(\pi, 0.3\pi)$  cut. (d) Dispersion extracted from a two-Lorentzian fit to the EDC data shown in (c). (e) EDC's at  $(\pi,0)$  and  $(0.9\pi,0)$  divided by the Fermi function (red circles) and a two-Lorentzian fit (blue lines). Inset: magnified region close to the chemical potential.

binding fits to the band dispersion extracted from the data. Panel (a) shows the Fermi surface contour for the moderately overdoped sample of  $T_c=80$  K. For this and lower doping levels, both sheets of the Fermi surface are hole like, as shown by previous studies. In the case of the heavily overdoped sample ( $T_c=55$  K), the bonding sheet of the Fermi surface remains hole like, but the antibonding Fermi surface becomes electron like and closes before it reaches the edge of the Brillouin zone, as illustrated in panel (b).

The finding that the Fermi-surface topology changes below the level of doping corresponding to  $T_c=55$  K has several important consequences. As the change of topology occurs in samples where  $T_c$  is still significantly high and is not associated with a rapid change of  $T_c$ , our results are not in support of those models of superconductivity which depend on the presence of a van Hove singularity. The relation of our finding to the question of quantum critical points in the phase diagram is a more subtle one. Anomalies in specific-heat data, which have been interpreted as due to the pseudogap

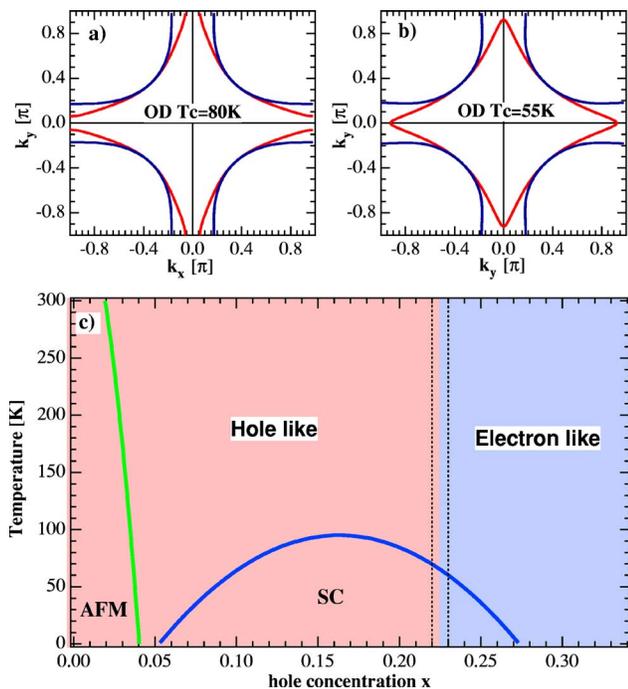


FIG. 4. (Color online) Fermi surface resulting from a tight-binding fit to data through the Brillouin zone. (a) For moderately overdoped samples with  $T_c = 80$  K. (b) For heavily overdoped samples with  $T_c = 55$  K. (c) Phase diagram with marked topology of the antibonding band. Dashed lines indicate uncertainty in the determination of the carrier concentration for the crossover in topology.

closing, occur at a doping value of 0.19 in this material,<sup>17</sup> considerably lower than the doping of approximately 0.225 we find our topology change to occur at.<sup>18</sup> On the other hand, our doping value does correspond to the one where collective effects were found to disappear (or at least significantly weaken) in the in-plane infrared conductivity.<sup>19</sup> And it is close to the value where  $c$ -axis transport indicates that  $T_c$  and the pseudogap temperature  $T^*$  merge.<sup>20</sup> It is interesting to note that in single-layer  $\text{Bi}_2\text{Sr}_2\text{CuO}_{6+\delta}$ , the topology change is near where  $T_c = 0$ ,<sup>11</sup> and there is evidence from NMR that

the pseudogap temperature merges with  $T_c$  at this doping as well.<sup>21</sup> As this is similar to our observation concerning the bilayer case, it implies that there may well be some connection between the pseudogap and the topology change of the Fermi surface.

One might also naively expect that a change of topology would affect transport properties, especially the Hall effect. However, the dependence of the Hall effect on doping is smooth in this range of doping.<sup>12</sup> This is not a surprise, though, since the Fermi velocity of the antibonding sheet is quite low in the  $(\pi, 0)$  region of the Brillouin zone. In support of this, tight-binding simulations we have made of the Hall effect find a hole like behavior for dopings far in excess of where the topology change occurs. Nevertheless, the presence of the van Hove singularity in the antibonding sheet very close to the chemical potential could have consequences for those properties which are sensitive to the breaking of particle-hole symmetry.

In summary, we report the observation of a change in the Fermi-surface topology in the heavily overdoped regime of  $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ . In overdoped samples, at dopings slightly below those corresponding to  $T_c = 55$  K, the antibonding band changes from hole like to electron like. The bonding band remains hole like over the whole doping range. This finding has potential consequences for theories of high-temperature superconductivity as well as the interpretation of transport measurements in this doping range.

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