Fermi Surface Topology of $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ at $h\nu = 33\text{eV}$: hole or electron-like?

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We present new results from Angle-Resolved Photoemission experiments (ARPES) on overdoped $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ (BSCCO) crystals. With greatly improved energy and momentum resolution, we clearly identify the existence of electron-like portions of Fermi Surface (FS) near $\bar{M}$ at $h\nu = 33\text{eV}$. This is consistent with previously reported data and is robust against various FS crossing criteria. It is not due to an artifact induced from $\vec{k}$-dependent matrix element effects. We also present evidence for a breakage in the FS pointing to the possible existence of two types of electronic components.

Angle-Resolved Photoemission Spectroscopy (ARPES) has become one of the most powerful tools for understanding the physics and electronic structure of high temperature superconductors (HTSC) and other correlated electron systems since it allows one to probe the energy and momentum relations directly. Over the past decade, major discoveries have been made on both the normal and superconducting states which include the Fermi Surface topology, superconducting gap symmetry, normal state pseudogap, etc.\cite{1}

Among the normal state properties, the Fermi Surface (FS) topology is one of the most important since it needs to be determined prior to correctly predicting many physical properties. Most of our information about the FS topology of HTSC’s has come from ARPES studies on BSCCO, and the results have been widely interpreted as a hole-like barrel centered around the ($\pi, \pi$) or X(Y) points of the Brillouin zone, as illustrated in figure 1(a)\cite{2,3}. This conclusion was made mainly by using incident photon energies around 21eV\cite{2,3}. Recently, we showed that the spectra and the physical picture appear quite different when measured using 33eV photons- there is a strong depletion of spectral weight around $\bar{M}$ ($\pi, 0$) and the FS appears to have electron-like portions, as illustrated in figure 1(b)\cite{4}. This result was later confirmed by Feng et al.\cite{5}.

This new interpretation of the data was questioned by two experimental groups in four recent papers\cite{6,7,8,9}. Fretwell et al. presented a detailed two-dimensional FS mapping on optimally doped BSCCO using 21.22eV photons. While their data gives perhaps the clearest evidence yet for the hole-like topology in this photon energy range, it does not address the different behavior observed at 33eV. Golden et al. did show a small portion of data at 33eV consistent with the data of Chuang et al.\cite{7}, and similar to Fretwell et al. and Mesot et al.\cite{8,9} they indirectly argued that this data was affected by unfavorable matrix element effects.

The experiments were done at Beaml ine 10.0.1 at the Advanced Light Source (ALS), Berkeley, CA using a Scienta SES 200 energy analyzer. We used the angle mode of the analyzer to simultaneously collect 89 individual spectra along 14° wide angular slices. We present 11 of these slices, representing almost 1000 individual energy distribution curves (EDCs) from one sample. The angular resolution along these slices was about $\pm 0.08^\circ$ in the $\theta$ direction and about $\pm 0.25^\circ$ in the perpendicular $\phi$ direction. At $h\nu = 33\text{eV}$, the converted momentum resolution is $(k_x, k_y) \approx (0.01\pi, 0.03\pi)$. We could map out the two-dimensional Brillouin zone by rotating the sample in either $\theta$ (parallel to the 14° slice) or in $\phi$ (perpendicular to the slice). The analyzer was left fixed with the central
analyzer angle making an 83° angle of incidence relative to the photon beam. In this configuration, the 14° slices are parallel to the incident photon polarization direction and the $\Gamma - \bar{M}$ high symmetry line.

The energy resolution was better than 10meV FWHM, as determined by the 10-90% width of a gold reference spectrum taken at 10K. The sample Bi046 used in this study was about 3mm on a side and was annealed in oxygen to over dope it, giving a $T_c = 79K$. Throughout the whole experiment, the base pressure was maintained below $4 \times 10^{-11}$ torr and the temperature was at 100K, well above $T_c$. All experimental data were normalized by using the high intensity emission above $E_F$, as discussed in reference [5].

Figure 2 shows the new data from this sample. The 11 panels of part (a) show false-color Energy Distribution Curves (EDC) taken at 2 different sets of $\theta$ angles (left and right panels) and 9 different $\phi$ angles. The vertical axes are the binding energy, and the horizontal axes are the $\theta$ angle along the 14° slice, with $0^\circ$ equal to normal emission. Each of the plots was normalized separately, i.e., the color scale can not be connected from one plot to another.

Each of these plots shows one or more features which disperse in energy as a function of angle (or wavevector $\vec{k}$). Most of these features can be easily followed up to $E_F$ at which point the features disappear due to the FS crossing. As a guide to the eye, we have overlaid a black curve on top of the data and labeled each features as S.S. (superstructure band) or M (main band). Due to polarization selection rules, the ARPES features along the $\Gamma - Y$ line have unfavorable emission such that in panels (ix)-(xi) the S.S. band has stronger intensity than the main band. In figures 2(b) and 2(c) we plot white dots which indicate the FS crossing points determined by looking at the dispersion in part (a), on the $\Gamma - \bar{M} - Y$ quadrant of the Brillouin zone. (The position of the 11 individual slices are indicated in panel (b),)

Another way to visualize FS crossings is to make a two-dimensional plot of the spectral intensity at $E_F$, i.e. $A(\vec{k}, E_F)$. This is plotted in parts (b) and (c) with data obtained by compressing the 11 panels of part (a). For these plots the relative intensity between each of the 11 panels is critical. They were first normalized by looking at the high-harmonic emission above $E_F$ only. We then integrated the spectral weight of the EDCs of Figure 2(a) over a 50meV energy window centered at $E_F$. Figures 2(b) and 2(c) show false color plots of this spectral intensity as a function of $\theta$ and $\phi$ with the color scale on the left. The FS should show up on this plot as the region of maximum spectral intensity.

The black lines in figure 2(b) show the experimentally determined FS from this data. The thick black lines represent the main FS in the first and second zones, while the thin lines represent the superstructure-derived FS, which is obtained by shifting the main FS by $(0.2\pi, 0.2\pi)$ along the $\Gamma - Y$ direction. These FS’s are consistent with the white dots obtained from panel (a) as well as with the high intensity locus of panel b. They also are consistent with the symmetrization method (figure 3(c)) and with the gradient or 50% point of $n(\vec{k})$ plots [5]. The FS determined here is qualitatively and quantitatively (to better than 5%) the same as that determined in reference [5]. The very slight shift of the high intensity locus away from $\bar{M}$ compared to the white dots is due to an effect of the finite energy integration window used to make the plot of panel (b) [5].

In contrast, the hole-like FS topology overlaid on the data in panel (c) cannot explain many of the crossing locations. This FS is taken from Fretwell et al, who also took data at 33eV [5]. The thick black line is the main FS while the thin black and red lines are the first and second order S.S. FS’s. The yellow lines are possible shadow bands obtained by reflecting the main and S.S. FS’s about the $(\pi, 0) - (0, \pi)$ line [5]. These FS’s show dashed sections which, as proposed by Fretwell, indicate a strongly reduced spectral intensity region due to strongly $\vec{k}$-dependent matrix element effects [5]. These are supposed to account for the lack of observation of a FS crossing from $\bar{M} - Y$. Even though this suggestion has many more free parameters than the electron-like topology of panel (b), it does not match the data as well. In particular it cannot match the curvature of the high intensity portion near $(\theta, \phi) = (14, 2)$ (also see cut (iii) in panel (a)) and it has trouble with the portion of the FS naturally explained by the S.S. band in panel (b) (the part circled in white). In the hole-like topology of figure 2(c) this would have to be explained by a combination of three bands - black, red, and yellow. The unlikeliness of this is amplified when a closer look at the EDC’s is taken. For example, panel (c) shows that the crossing at $(\theta, \phi) = (19, 5)$ should come from the yellow shadow band. As such it should have reversed E vs. $\vec{k}$ dispersion from the main band, while panel (vi) of part (a) shows that it does not. The experimental intensity is also too strong - it should be a shadow of a S.S. band and should also be strongly reduced by matrix element effects (dashed lines).

The 33eV FS plots presented by Fretwell et al. [5] are quite similar to the data in figure 2, one of which is reproduced in figure 3. Panel (a) shows their data and their interpretation within the hole-like FS topology. The image plot was obtained by integrating the spectral weight over the relatively large energy window $(-100meV, 100meV)$ in the superconducting state at 40K. We feel that the hole-like topology presented in this figure has a number of deficiencies and can not explain the data well. First, the hole-like FS segments extend towards $\bar{M}$ while the data does not. Fretwell et al. attempted to reconcile this by empirically introducing a strongly $\vec{k}$-space dependent ma-
trix element effect to drastically reduce the weight near $M$. However such an effect cannot explain the curvature of the FS which is manifested in the intensity plot by the locus of high intensity points. Namely, in figure 3(a) we have circled a high intensity region which cannot be explained by a hole-like FS. Figure 3(b) shows the electron-like FS (thick white line) plus S.S. band portions (thin white lines) overlayed with the same intensity plot. Now the main band FS trace matches beautifully with the locus of high intensity spots, without having to introduce any complicated matrix-element dependent physics.

The S.S. band circled in our figure 2(b) is not apparent in Fretwell et al.’s data of figure 3(a) and (b). We suggest two possible reasons for this discrepancy: (1) the S.S. bands may be weaker in Fretwell’s data, or (2) they perhaps did not include enough dynamic range in their color scale plot, so that the S.S. bands were not apparent.

Using symmetrized EDC’s, Mesot et al. also argued that their 34eV data from overdoped $Bi_2Sr_2CuO_{6+δ}$ supported the hole-like topology since they did not observe a FS crossing along $Γ-M$ but they did observe one along $M-Y$. We have applied this method to our data, and find that it is supportive of an electron-like topology, as shown in figure 3(c). Each EDC was added to a mirror image of itself reflected around $E_F$, which assuming electron-hole symmetry near $E_F$ will remove the effect of the Fermi function cutoff. As stressed by Mesot, the symmetrized EDC will show a peak at $E_F$ if there is a FS crossing, otherwise it will show a dip. Figure 3(c) shows the symmetrized EDC along $Γ-M-Z$ from the data of figure 2. The dip at $E_F$ disappears at around angle $(θ, φ) = (15, 0)$, indicating the FS crossing - a location that agrees to within 2% with that obtained directly from figure 2. The consistency of the results obtained by all methods (see also references 5 and 6) gives us confidence in the electron-like topology observed at $hν = 33eV$. However, we still need to worry about the different result obtained by Mesot et al. The difference might be due to an incorrect determination of $E_F$ since the symmetrization method is very sensitive to a shift of $E_F$. We have performed symmetrizations on BSCCO data from three different experimental systems and from both the single layer and double-layer compounds. All data from over or optimally doped samples have given the same result - a peak at $E_F$ after symmetrization, indicating a FS crossing along $Γ-M$. This gives us confidence that an undetected $E_F$ calibration error could not have adversely affected our data.

The increased energy and momentum resolution obtained in figure 2 brings up other subtleties which have not been previously observed. If we track the main electron-like FS from the $Γ-Y$ line towards the $Γ-M$ line, the intensity first gets greater, which is understood due to polarization effects (12). It then gets weaker around $(14, 2)$ before getting stronger again along the $Γ-M$ line. This makes the FS appear as if it has two components - one nearer the $Γ-Y$ line and one nearer the $Γ-M$ line. Further study needs to be carried out to deconvolve the origin of the separation of the FS into these components, as well as to study potential differences in the behavior of each component.

Finally, of course, there is the critical issue of connecting the electron-like FS topology observed at 33eV with other topologies observed at other photon energies. A natural possibility is to consider coherent three-dimensional band structure effects from the $x^2-y^2$ band (or from the $s^2$ band (12)), although this would need to be reconciled with the highly two-dimensional nature of the cuprates. Even-odd splitting between the $CuO_2$ bilayer may produce both an electron and a hole like FS in the same sample, although this would need to be reconciled with the single-layer $Bi2201$ data which also appears to show both topologies (1). Two FS’s may simultaneously exist in the same sample for other reasons as well, for instance due to phase separation into hole-rich and hole-poor regions or into regions with and without stripe disorder (1), each of which may produce its own FS portions. Within these scenarios we still need to understand why one piece of the FS is accentuated at one photon energy while another is accentuated at another. Matrix element effects may play a role in this (13).

In this communication we have presented high energy and momentum resolution ARPES results on the normal state of overdoped $Bi_2Sr_2CaCu_2O_{6+δ}$ at $hν = 33eV$. We clearly identify the existence of electron-like portions of Fermi Surface near $M$ by looking at the high intensity locus in $A(\vec{k}, E_F)$ plots, dispersion of EDCs, and symmetrized EDCs. We reach the same result by looking at either the main band or the S.S. bands. In contrast, the hole-like topology cannot explain the details of the spectra, even with the ad-hoc inclusion of strong $\vec{k}$-dependent matrix element effects. In addition, our increased resolution shows some new and potentially important subtleties of the data including a break in the main FS.

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FIG. 1. Hole-like FS topology (a) versus electron-like topology (b).

FIG. 2. (a) E vs. $\vec{k}$ plots from overdoped Bi2212 sample Bi046 measured at 100K. Vertical axes are binding energy (eV) and horizontal axes are the angle $\theta$. The right panels are centered at $\theta = 18^\circ$, while the left panels are centered at $\theta = 8^\circ$. The location of each cut is shown in panel (b). The color scale is shown at the top left corner, with larger value (1.0) indicating more spectral weight. Black lines indicate the E vs. $\vec{k}$ dispersion relation and are guides to the eye. The FS crossing points are determined by looking at the intersection of the guide lines and $E_F$ and are labeled S.S. (superstructure band) and M (main band). Panels (b) and (c) are plots of the spectral intensity at $E_F$. White dots are the FS crossings from part (a). Panel (b) shows the agreement with the electron-like topology while panel (c) shows the disagreement with the hole-like topology.

FIG. 3. (a) Data from Figure 1(c) of Fretwell et al.[6] The circled region cannot be explained by the the hole-like FS topology. (b) Same data overlayed by a FS with electron-like portions (white). (c) Symmetrized EDCs along $\Gamma - \bar{M}$ for a variety of $\theta$ angles, with $\phi=0$. The first peak at $E_F$ shows up at $(15,0)$, indicating a FS crossing.