How different Fermi surface maps emerge in photoemission from Bi2212

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Abstract

We report angle-resolved photoemission spectra (ARPES) from the Fermi energy ($E_F$) over a large area of the ($k_x,k_y$) plane using 21.2 eV and 32 eV photons in two distinct polarizations from an optimally doped single crystal of Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ (Bi2212), together with extensive first-principles simulations of the ARPES intensities. The results display a wide-ranging level of accord between theory and experiment and clarify how myriad Fermi surface (FS) maps emerge in ARPES under various experimental conditions. The energy and polarization dependences of the ARPES matrix element help disentangle primary contributions to the spectrum due to the pristine lattice from those arising from modulations of the underlying tetragonal symmetry and provide a route for separating closely placed FS sheets in low dimensional materials.

Establishing the nature of the Fermi surface (FS) in the metallic state—the shape, size, connectivity and the number of FS sheets \cite{1,4} and the character of states at and near the Fermi energy ($E_F$), is crucially important for identifying the correct superconducting scenario in the cuprates. In this connection, high-resolution angle-resolved photoemission spectroscopy (ARPES) provides a unique window in low dimensional materials. However, even under identical conditions of doping, temperature and other physical parameters, the imprint of the FS in ARPES often varies dramatically with the energy and polarization of the incident photons. This article reports fundamental progress in understanding this remarkable behavior by considering the example of Bi2212 which has played the role of a touchstone and a workhorse in ARPES studies of the high-Tc’s. By comparing ARPES measurements over a large area of the FS with corresponding first-principles simulations, we show how myriad tapestries of FS maps originate in photoemission, and how the ARPES matrix element blends and highlights various parts of the electronic spectrum—pristine states, effects of modulations \cite{5-10}, different FS sheets and the like, depending upon the specifics of the photon energy and polarization.
High quality single crystals of optimally doped Bi2212 ($T_c=90$ K) were grown by the traveling solvent floating zone method. The FS maps were produced by measuring the photointensity within a narrow energy window at $E_F$ over the full 360° angular range in the $(k_x,k_y)$ plane at the SU8 high-resolution beamline of the Super-Aco synchrotron ring at LURE. The data were collected on a regular mesh in polar ($\theta$) and azimuthal angles ($\phi$) of steps $\Delta\theta = 1^\circ$, $\Delta\phi = 1^\circ$. Some measurements employed He-I light (unpolarized) from a He discharge lamp. The overall energy resolution varied from 12 meV to 60 meV depending on measurement conditions. Procedures to assure accurate sample alignment included a complete set of photoelectron diffraction azimuthal and polar scans of the Bi core level in the high-energy regime which were recorded in situ in order to define the $\bar{\Gamma}$ point and the main high symmetry directions. Two different detection geometries – referred to as ‘even’ and ‘odd’ – have been employed to obtain the ARPES spectra. In the even case, the detector is constrained to move in the horizontal plane, which is the same as the plane of the incident light, whereas for the odd case, the detector is chosen to move in the vertical plane. The polarization is defined as measured with respect to radial lines through $\Gamma$: even (odd) polarization implies the polarization vector lies along (transverse to) this radial direction. It can then be shown that when emission from a mirror plane in the crystal lattice is involved (e.g. along the $\Gamma - M$ line), the even (or odd) experiment only probes initial states of even (or odd) symmetry. In the case of emission from the Cu-O planes in Bi2212, the relevant initial states are predominantly Cu $3d_{x^2-y^2}$ hybridized with O $2p_{x,y}$ and states along the $\bar{\Gamma} \rightarrow \bar{M}$ line (along the Cu-O-Cu bonds) are expected to be intense in the even experiment, while states along $\bar{\Gamma} \rightarrow \bar{X}(\bar{Y})$ will be strong in the odd measurements (since deviations from tetragonal order are small).

All computations in this article are based on the one-step model of photoemission extended to treat arbitrarily complex unit cell materials. Effects of multiple scattering and the ARPES matrix element are thus included realistically in the presence of a specific surface termination, taken here to be the Bi-O layer. The finite lifetimes of the initial and final states are incorporated by giving suitable imaginary parts to the self-energies of the associated initial and final state propagators. The crystal potential was obtained via a selfconsistent KKR procedure assuming a perfect tetragonal lattice which yielded the well-known LDA-based band structure and FS of Bi2212. The actual potential used in this work however has been modified slightly such that the Bi-O pockets around the $M$-point are lifted above $E_F$ to account for their absence in the experimental ARPES spectra. A number of simulations have also been carried out where repulsive barriers were placed between the two CuO$_2$ planes in the Ca layers in order to mimic correlation effects beyond the LDA which are expected to reduce the bilayer splitting. Finally, in order to describe the effects of the orthorhombic modulation and the $\sim (1 \times 5)$ superstructure present in Bi2212, we have taken the spectrum computed for the tetragonal case and superposed on this the same spectrum with appropriate weights after suitable translations in the reciprocal space. The weights estimated from relative intensities in the experimental FS maps are summarized in Table 1 and described in the text below.

Figure considers two sets of theoretical spectra at 21.2 eV in the even and odd detection geometries for the pristine tetragonal lattice, and helps set the stage for our discussion. The right hand Figs. (b,d) refer to simulations where the bilayer splitting has been artificially reduced to a near zero value and both FS sheets are hole-like around the $\bar{X}(\bar{Y})$ symmetry
point. The case with a bilayer splitting of $\sim 200$ meV where the first FS sheet is hole-like and the 2nd sheet is slightly electron like is depicted in the left hand Figs. 1(a,c). We see by comparing Figs. 1(a) and 1(b) that there is a striking increase in the intensity around the $\bar{M}$-point for even detection due to the presence of the aforementioned 2nd underlying FS sheet. In fact, we have carried out numerous other simulations in which the size of the bilayer splitting and/or the position of $E_F$ around the $\bar{M}$-point was varied; these results show clearly that about the only way in which one can obtain a large intensity around the $\bar{M}$-point in the even detection geometry for 21.2 eV photons is when there is an additional band present very close to $E_F$ around the $\bar{M}$-point. This is a crucially important observation which we will recall below in analyzing the experimental data. Fig. 1 also highlights the differences between the even and odd maps more generally. The 2nd FS sheet so prominent in the even map of Fig. 1(a) is essentially ‘invisible’ in the corresponding odd map of Fig. 1(c). Also, the odd map is complementary to the even map in the sense that regions of high intensity in one map are often replaced by those of low intensity in the other and vice versa.

The determination of the FS topology of the underlying pristine phase in Bi2212 has been complicated by the presence of secondary features tied to superlattice and shadow bands. The results of Table 1 offer insight into how a headway can be made in disentangling primary and secondary features by exploiting the energy and polarization dependences of the ARPES matrix element. We see that in the 21.2 eV even geometry, no secondary feature displays a weight greater than 20 % of the primary features, and therefore, this energy and polarization is well-suited for delineating the primary FS. In sharp contrast, the weights of secondary features are significantly greater at 32 eV in both the even and odd spectra as well as in the 21.2 eV odd spectrum. Interestingly, the shadow feature is most prominent in the 32 eV odd case, and the second superlattice image is visible in 32 eV even map, albeit weakly.

Although absolute intensities are not our focus, one aspect of these is particularly germane to this discussion. The theoretically computed maximum absolute ARPES intensities of the primary features are in the ratios: 21.2 eV (even): 21.2 eV (odd): 32 eV (even): 32 eV (odd) = 5:2:1.2:0.7, in reasonable accord with the corresponding experimental values of: 5:1.7:0.8:0.6, uncertainty in determining absolute experimental intensity notwithstanding. Applying these ratios to the data of Table 1 [which gives the relative weights of the secondary features], it is found that the absolute intensities of various secondary features are not all that different at the two photon energies considered for either the odd or the even maps. In other words, the primary emissions become highlighted in the 21.2 eV even measurements not because the secondaries are weak, but due to the primaries becoming much stronger.

Figures 2 and 3 compare experimental and theoretical spectra at 21.2 eV and 32eV respectively. While changes in the ARPES maps of the FS with photon energy and polarization are striking, an excellent overall agreement with theory is seen in all cases. The unpolarized (He I) data (Fig. 2(a)) and theory (Fig. 2(b)) both show a clear imprint of the large hole sheet centered around $\bar{X}$ or $\bar{Y}$, but relatively little trace of the 2nd FS sheet around $\bar{M}$. However, under even polarized light (Figs. 3(c,d)) this 2nd sheet comes alive giving intense emission around the $\bar{M}$-points. As emphasized already in connection with Fig. 1 above, the appearance of this large intensity is an unmistakable signature of the presence of a second band lying close to $E_F$ at $\bar{M}$. As noted above, under these experimental conditions secondary features are quite weak (Table 1) and can be ignored in the analysis of Figs. 2(c,d). We
see thus how a systematic comparison between experimental and theoretical ARPES maps shows that the 21 eV even detection geometry is well suited for establishing unambiguously the presence of the second FS sheet with negligible interference from umklapps and shadow bands.

Under odd polarization (Figs. 2(e,f)) secondary features develop greater relative intensity, so the even and odd maps look quite different. As expected, the emission around \( \bar{M} \) from the 2nd sheet is suppressed in this polarization. On the other hand, the trace of the FS sheets is reinforced along the lattice modulation direction via superposition with its Umklapp images, thereby distorting the image of the hole sheet in the odd map (Fig. 2(e)), so that caution must be exercised in deducing physical parameters (size and shape) from this spectrum. The mix of primary and secondary features is quite different in the 32eV data, Fig. 3, even though some of the characteristics are basically similar. For example, the 2nd FS sheet is emphasized in the even polarization in Figs. 3(a,b), but suppressed in the odd case of Figs. 3(c,d). Compared to 21.2 eV, there is generally a greater spectral weight at higher momenta; for example, the image of the 2nd sheet is more or less equally intense in the 1st and 2nd BZ’s in Figs. 3(a,b), but in the 21.2 eV Figs. 3(c,d), the 2nd BZ imprint is quite weak in relation to that in the 1st BZ. The combination of the two FS sheets with appropriately weighted secondary images yields two nearly parallel bands of intense emission which are oriented along the \((\pi, -\pi)\) direction in Fig. 3 and appear quite striking. Interestingly, in even polarization (Figs. 3(c,d), or 3(a,b)) the spectra show a remarkable line of essentially zero intensity along the \( \bar{\Gamma} \rightarrow \bar{Y} \) direction, as expected for a mirror plane. Along the perpendicular line \( \bar{\Gamma} \rightarrow \bar{X} \), there is clear residual intensity – a signature of superlattice effects which break the symmetry selection rules.

In conclusion, we demonstrate that dramatic differences in the observed FS maps under various experimental conditions arise as a consequence of the ARPES matrix element which gives the primary FS features (arising from the pristine lattice) a weight which depends upon the energy and polarization of light in a very different manner from that of the secondary features associated with the superlattice and orthorhombic modulations. In this way the ARPES matrix element helps disentangle various aspects of the electronic structure and fermiology of this complex system. In particular, we confirm recent reports \[2\] of two FS sheets in Bi2212, extending the result to optimal doping. There is one large hole-like standard sheet and a second electron-like sheet which arises from a band which lies very close the Fermi energy at the \( \bar{M} \)-point. The wide ranging accord between theory and experiment suggests that the band theory framework implicit in our computations captures the essential underlying physics. If so, the two FS pieces should be viewed as the result of conventional bilayer splitting. However, it would be wise to keep the door open for admitting other explanations, e.g. some form of a nano-scale phase separation or stripe order.

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TABLE I. Relative fractional weights of various secondary features in Bi2212 obtained by analysing the experimental FS maps where the primary spectrum for the pristine lattice is normalized to unity. The superlattice modulation gives the 1st and 2nd Umklapp images, while the orthorhombic modulation yields the shadow feature and the related Umklapps. The translation vectors involved are of form $\eta(\pi, \pi)$ parallel to the orthorhombic $b^*$ axis. Listed values of $\eta$ come in pairs. 1st and 2nd Umklapps roughly correspond to $\eta$ values of $\pm 1/5$ and $\pm 2/5$, respectively.

| $\hbar \nu$ | detection geometry | orthorhombic modulation | superlattice modulation |
|-------------|---------------------|-------------------------|-------------------------|
|             | shadows             | $1^{st}$ umklapps        | $1^{st}$ umklapps        |
| 21.2 eV     | even                | 0.10                    | 0.20                    |
|             | odd                 | 0.30                    | 0.40                    |
| 32 eV       | even                | 0.15                    | 0.35                    |
|             | odd                 | 0.40                    | 0.40                    |
| $\eta$ [Translation vector is $\eta(\pi, \pi)$] | $\pm 0.5$ | $+(0.5\pm 0.21)$ | $\pm 0.21$ | $\pm 0.42$ |
Figure Captions

Fig. 1
Theoretical maps at 21.2 eV for emission from $E_F$ in pristine (tetragonal) Bi2212 for even and odd polarizations of light described in the text. The left hand simulations (a,c) refer to the band theory-based crystal potential with a bilayer splitting of $\sim 200$ meV at the $\bar{M}$ point. In the right hand side simulations (b,d), the bilayer splitting has been artificially reduced to a nearly zero value. Intensities are normalized to the same value in all maps and plotted in hot colors (whites and yellows are highs) on a linear scale. The square in solid white lines marks the 2D Brillouin zone.

Fig. 2
Theory and experiment are compared directly at 21.2 eV for even and odd polarizations, as well as for the unpolarized He I light. Effects of superlattice and orthorhombic modulations are included in theory as discussed in the text. See caption to Fig. 1 for other pertinent details.

Fig. 3
Same as Fig. 2 except that this figure refers to 32 eV synchrotron light.
FIGURES

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