

Polarization selection rules and superconducting gap anisotropy in $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$

M. R. Norman and M. Randeria

Materials Science Division, Argonne National Laboratory, Argonne, Illinois 60439

H. Ding, J. C. Campuzano, and A. F. Bellman

*Materials Science Division, Argonne National Laboratory, Argonne, Illinois 60439
and Department of Physics, University of Illinois at Chicago, Chicago, Illinois 60607*

(Received 10 July 1995)

We discuss polarization selection rules for angle-resolved photoemission spectroscopy in Bi2212 . Using these we show that the hump in the superconducting gap observed in the X quadrant in our earlier work is not on the main CuO_2 band, but rather on an umklapp band arising from the structural superlattice. The intrinsic gap is most likely quite small over a range of $\pm 10^\circ$ about the diagonal directions.

Recently, our group, by use of angle-resolved photoemission spectroscopy (ARPES) on high quality single crystals, has found that the superconducting gap in Bi2212 has a non-trivial momentum dependence.¹ In particular, the gap is suppressed over a range of $\pm 10^\circ$ about the diagonal directions (at 45° to the CuO bond directions) of the square lattice zone [for Bi2212 , these directions are ΓX and ΓY where $X \equiv (\pi, -\pi)$ and $Y \equiv (\pi, \pi)$]. In addition, though, we found that the gap was actually nonzero over this range, with a weak maximum along the diagonal and two nodes 10° on either side (i.e., a hump). The simplest interpretation of such data is that the order parameter has anisotropic s -wave symmetry.² Such an order parameter would not be in conflict with experiments which only probe the existence of nodes, but it would be in conflict with phase coherence experiments on Y-Ba-Cu-O which reveal a sign change of the order parameter under rotation by 90° ,³ although similar experiments have not been performed on Bi2212 .

A striking point about our data was that the hump in the gap along the diagonal was less pronounced in the Y quadrant of the zone (Fig. 1) than the X quadrant (Fig. 2).⁴ This led to a potential concern about the interpretation of the data because of the presence of an incommensurate superlattice in Bi2212 with a \vec{Q} of $(0.21\pi, 0.21\pi)$ which makes the X and Y quadrants inequivalent.⁵ This superlattice leads to the presence of $\pm \vec{Q}$ umklapp bands in the ARPES data.^{1,6} Because \vec{Q} is along ΓY , these umklapp bands are well separated from the main band near the diagonal direction in the Y quadrant, but since \vec{Q} is perpendicular to ΓX , the two umklapp bands are predicted to be quite close to the main band near the diagonal direction in the X quadrant, and thus should be hard to resolve (Fig. 3).¹ In fact, the main band and superlattice band are predicted to cross at exactly the same location as where the nodes in the gap were observed in the X quadrant (Fig. 3). This suggested the possibility that the hump in the gap in the X quadrant was a consequence of being on the superlattice band instead of the main band. In an earlier paper of ours,² we demonstrated that even if the main band had a gap with d -wave symmetry, the observed gap in the X quadrant could indeed have this hump, simply because the superlattice band along the diagonal direction corresponds to

a location on the main band about 20° away. There were two problems with such an interpretation. The first was why only the superlattice lattice band was observed near the diagonal in the X quadrant and not the main band. The second was that a similar (but smaller) "hump" was observed in the Y quadrant, where these arguments do not apply (that is, the

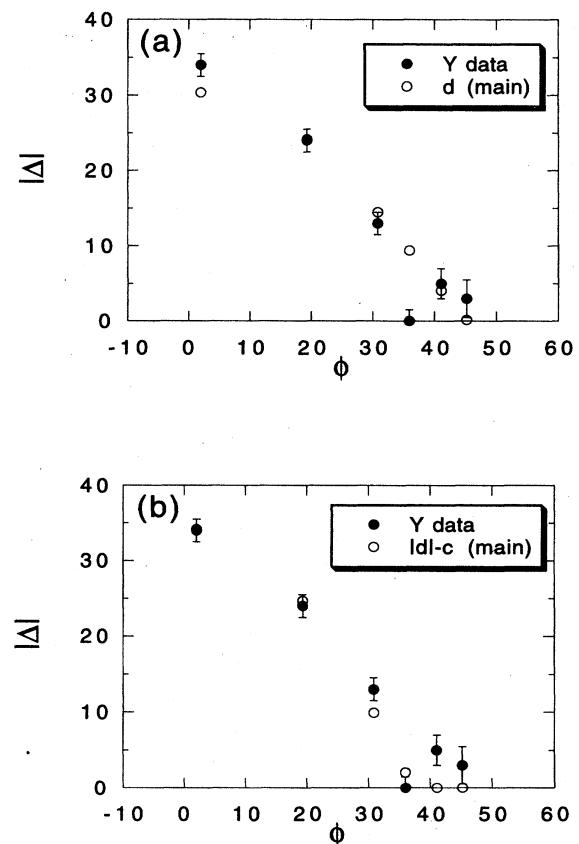


FIG. 1. Gap in meV in the Y quadrant versus angle (in degrees) on the Fermi surface (filled circles) with fits to the data using (a) a d -wave gap and (b) a $|d|-c$ gap (open circles).

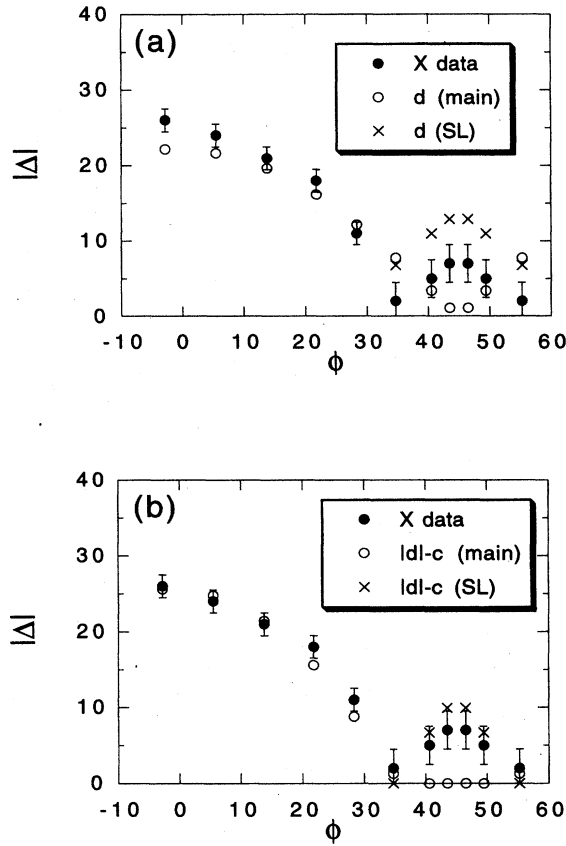


FIG. 2. Gap in meV in the X quadrant versus angle on the Fermi surface (filled circles) with fits to the data using (a) a d -wave gap and (b) a $|d| - c$ gap [open circles for the main band, crosses for the superlattice (SL) band nearest the main band].

observed gap was definitely on the main band, as seen in Fig. 3).

As it turns out, the resolution of the first problem was essentially present in the original data and not realized at the time. We note that the data in the X quadrant were taken with a polarization vector along the ΓX direction (Fig. 2 of Ref. 1). Now, ΓX is a symmetry line of the zone (this direction is reciprocal to the orthorhombic a axis of Bi2212), and therefore, bands must be even or odd relative to reflections about this line. As the band contains copper states of $d_{x^2-y^2}$ symmetry, the main band must be odd relative to this line. Since the polarization vector is along this line, then the dipole matrix element vanishes and therefore emission from the main band cannot be observed. Now, consider the two superlattice bands which cross each other along ΓX (Fig. 3). One can make a linear combination of these two bands at the crossing point. The combination $\psi(\vec{k} + \vec{Q}) + \psi(\vec{k} - \vec{Q})$ has odd symmetry, like the main band, and thus should not be observed either. The combination $\psi(\vec{k} + \vec{Q}) - \psi(\vec{k} - \vec{Q})$, though, has even symmetry, and is maximally enhanced in this polarization geometry. Therefore, the observed gap near the diagonal in the X quadrant must be on the even symmetry combination of the superlattice bands, and thus, as conjectured in the previous paragraph, the hump in the gap is a superlattice effect.

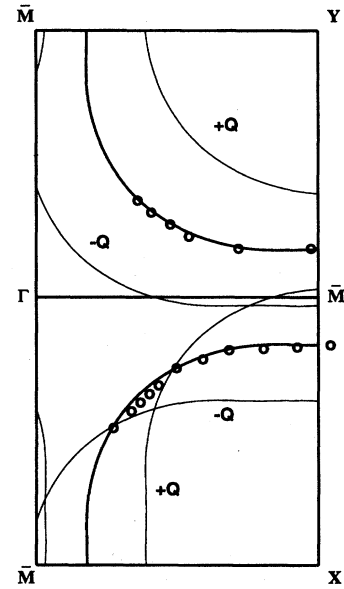


FIG. 3. Fermi surface from a tight binding fit to the energy dispersions in the X and Y quadrants of the zone. The thick line is the main band, the thin lines the superlattice bands (marked $+Q$ and $-Q$). The data points at which the gap was measured are shown as open circles.

To explicitly demonstrate this, we have looked at two models for the gap function. The first is the standard d -wave gap $d \equiv \cos(k_x + q) - \cos(k_y + q)$ where q is 0 for the main and $\pm 0.21\pi$ for the superlattice bands. The other is $\max(|d| - c, 0)$ where c is a constant, which was designed to have an angular range with zero gap. The data are then fit assuming the four or six data points nearest the diagonal are on the superlattice band.⁷ The resulting gaps are plotted along the main and superlattice sheets in Fig. 2 (note from Fig. 3 that data for angles less than 35° are definitely on the main band). The comparison to experiment is quite reasonable, especially in the case of the $|d| - c$ gap (its rms error in the X quadrant is less than half that of the d -wave gap⁸). The same also applies in the Y quadrant as seen in Fig. 1. In fact, both fits have a smaller rms error in the Y quadrant than the $\cos(k_x)\cos(k_y)$ function previously used to describe a hump in the gap.² We also note that the angular range of zero gap for the $|d| - c$ model is compatible with NMR data on samples from the same source as ours, which reveal the presence of a residual density of states about 24% of the normal state value.⁹

The observation that the hump in the X quadrant is a superlattice effect also explains a number of other puzzling results. First, the two spectra nearest ΓX had leading edge slopes which were not resolution limited.¹ This can be understood now since the \vec{k} vectors at which this data were taken corresponded to an energy near the Fermi energy of the main band but below the Fermi energy of the superlattice bands (Fig. 3). Second, previous data¹⁰ indicated a strong polarization dependence of the photoemission intensity along the diagonal in the Y quadrant but a weak one in the X quadrant. In particular, the intensity essentially vanished for

polarization parallel to ΓY in the Y quadrant. This result is expected since both main and superlattice bands are odd relative to ΓY (since \vec{Q} is along ΓY). In the X quadrant, though, when the polarization is perpendicular to ΓX , the main band and odd symmetry combination of the superlattice bands should be observed, whereas when the polarization is parallel to ΓX , only the even symmetry combination of the superlattice bands should be observed. Our data in the normal state¹¹ indicate that the odd symmetry combination is not observed, perhaps due to final state effects. Therefore, if the main and even symmetry combination of the superlattice bands have comparable intensities, then a weak polarization dependence should be observed in the X quadrant. As a corollary, the hump in the X quadrant should disappear if the polarization is perpendicular to ΓX . Data by our group indeed support this picture.

This now leaves the remaining problem to be resolved: the observation of a hump in the Y quadrant. This hump was based on the two data points nearest ΓY (Fig. 1). We note, though, that the error bars of Ref. 1 are consistent with a zero gap for the data point along ΓY . We have gone back and reanalyzed the data for the other point and still conclude that the optimal fit has a gap of order 5 meV, and thus not consistent with zero. We are hesitant, though, to attach too much significance to data at a single point, and therefore conclude that the current data set is not extensive enough to definitively prove the existence of a hump in the Y quadrant. We caution that the data in the Y quadrant were taken in steps of $\sqrt{2}^\circ$ in photoemission coordinates, which along the diagonal corresponds to an energy change (from fits to the dispersion) of over 80 meV per step. Although the momentum windows of the data points do overlap with one another (since the window has a radius of 1°), the resolution normal to the Fermi surface is still not as high as one would like. In the future, it would be desirable to perform experiments using smaller step sizes and higher momentum resolution. Second, the data fits were based on a spectral function which only has resolution broadening with other effects being absorbed into a model background function. The actual spectral function has a strongly energy dependent line shape due to self-energy effects. In the superconducting state, though, the line broadening will be suppressed for frequencies below 3Δ if it is due to electron-electron scattering,¹² and such a model appears to be consistent with our data since the slopes of the leading edge are resolution limited, even along the diagonal. Since it is a fit to the leading edge which deter-

mines the gap, then ignoring the detailed energy dependence of the broadening should be valid, but one always worries that a more sophisticated model of the line shape taking into account its frequency dependence (which would necessitate using a different background function) might yield different estimates of the gap.

Given the above, the existence of a hump in the intrinsic gap is questionable. While a hump necessarily implied anisotropic s -wave pairing, an extended region of zero or small gap could be consistent with a number of models.¹³ One of these might be dirty d wave, with the gap suppressed in a large angular range about the diagonal due to impurity scattering. The NMR data previously mentioned were interpreted in terms of this model.⁹ There is a problem with such a scenario. Gaplessness due to dirt shows up in the spectral function as a low frequency tail.¹⁴ In ARPES, though, the gap is determined by measuring the shift in the leading edge of the spectrum, and this shift should be relatively unaffected for small concentrations of impurities.¹⁵ If we assume, then, that the suppressed gap region is not due to dirt, then another possibility is a d -wave gap, but not of the simple $\cos(k_x) - \cos(k_y)$ form.⁸ Since this simple form will occur for short-range interactions, the implication then is that the interaction must be long range to obtain a gap similar to what is observed. The same argument would also apply to anisotropic s -wave models (thus phase coherence experiments would be necessary to determine the actual symmetry of the order parameter). In fact, we know of two such models which can give gaps of this form: the interlayer tunneling model of Chakravarty *et al.*¹⁶ and the poorly screened electron-phonon model of Abrikosov.¹⁷ Both of these models have the property that they are local in \vec{k} space and thus long range in real space.

In conclusion, a reanalysis of our data using polarization selection rules has led us to conclude that the actual gap in Bi2212 is suppressed over a $\pm 10^\circ$ range about the diagonal, although more experiments at better momentum resolution will be necessary to completely resolve this issue. Such a suppressed gap region could be either due to dirt or to a pairing interaction long range in space. Further experiments on samples with controlled defect densities could be used to differentiate between these two scenarios.

We would like to thank Phil Anderson and Roland Fehrenbacher for useful discussions. This work was supported by the U. S. Department of Energy, Basic Energy Sciences, under Contract No. W-31-109-ENG-38.

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⁴Although the data in the X and Y quadrants were taken on different samples, all photoemission groups consistently report a larger gap along the diagonal in the X quadrant than the Y quadrant.

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⁶J. Osterwalder *et al.*, Appl. Phys. A **60**, 247 (1995).

⁷Two of the data points in the X quadrant are close to the crossing of the main and superlattice bands, so it is unclear which band to assign them to. For the same reason, though, it makes little difference in the fits whether they are assigned to one or the other.

⁸A gap which is the square of the d -wave gap has the lowest rms error of any single function fit we have looked at, with an error only slightly larger than that of the $|d| - c$ gap (the latter having two fit parameters). A gap of this type has been suggested by P. W. Anderson.

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