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Mohit Randeria
Materials Science Division
Argonne National Laboratory
Argonne, IL 60439
and
Theoretical Physics Group
Tata Institute of Fundamental Research
Bombay 400005, India

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Materials Sciences Division, Argonne National Laboratory, Argonne, IL 60439, USA

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Theoretical Physics Group, Tata Institute of Fundamental Research, Bombay 400005, India

Abstract

Recent angle-resolved photoemission (ARPES) studies of the high T_c superconductors by the Argonne group are briefly reviewed. First we discuss sum rules to establish a spectral function interpretation of the data, and the use of ARPES to obtain the momentum distribution. We then apply these ideas to the normal and superconducting state spectra for $Bi_2Sr_2CaCu_2O_8$. Among the topics discussed are the Fermi surface, polarization selection rules, bilayer splitting and the superconducting gap.

Key words: photoemission, high temperature superconductors

1. Introduction

Starting with the pioneering work of Olson and collaborators [1] angle-resolved photoemission spectroscopy (ARPES) has played a major role in the study of the high temperature superconductors (HTSC) [2]. Among the important early results obtained by ARPES are: observation of the superconducting gap, and of a normal state with a Luttinger Fermi surface and extended saddle-point singularities in the band structure.

In this paper I briefly review some recent insights gained from ARPES studies of the HTSC in collaboration with Juan-Carlos Campuzano, Hong Ding, and Michael R. Norman.

Much of the material covered in my Erice lecture is by now available in the literature, I will therefore only mention the main ideas, give the relevant references, and present an informal discussion to complement these references. For lack of space, I will refer to the figures in the original papers.

2. What does ARPES measure?

There are several reasons for the great success of ARPES for the high T_c materials. First, the great improvement in the experimental (especially energy) resolution allows one to study spectral features on the scale of the SC gap in these materials. Second, the natural cleavage plane in Bi2212 leads to extremely smooth surfaces, which is crucial for the success of this surface-sensitive technique. Finally, the quasi-two-dimensionality of the electronic structure permits one to unambiguously determine the momentum of the initial state from the measured final state momentum. Further, the quasi-2D property may also play an important role in being able to ignore the final state broadening effects [3].

Nevertheless, the theoretical interpretation of ARPES spectra is, in general, quite difficult since photoemission formally measures a *nonlinear* response function [4]. The photoelectron current at the detector is proportional to the number of incident photons, i.e., to the *square* of the vector potential, and the relevant correlation function is a three current correlation. Under certain simplifying conditions, principally the validity of the impulse (or sudden) approximation, this reduces to a much simpler result involving only the one-particle spectral function $A(\mathbf{k},\omega)$. While this simplification is often taken for granted, it is not at all clear *apriori* that for ultraviolet spectroscopy, with 15 - 30 eV incident photons, whether the sudden approximation should be valid: the outgoing photoelectron is not obviously so energetic that its interaction with the photohole may be simply ignored. (A more detailed discussion based on the many-body effects in the three current correlation will be presented elsewhere).

Recently we have gained confidence in the validity of the spectral function interpretation using the following strategy [5]. Let us assume that the sudden approximation is valid, deduce some general consequences (sum rules), and then test those experimentally. One can

show that the ARPES intensity is then given by

$$I(\mathbf{k},\omega) \propto |\langle\psi_f|\mathbf{p}\cdot\mathbf{A}|\psi_i\rangle|^2 f(\omega)A(\mathbf{k},\omega) \tag{1}$$

where the first factor is the dipole matrix element, f is the Fermi function, and $A(\mathbf{k},\omega)$ is the initial state (or "photohole") spectral function. The selection rules arising from the matrix element will be discussed later.

We first discuss the line-shape of the energy distribution curve (EDC) and its temperature (T) dependence which is controlled by $f(\omega)A(\mathbf{k},\omega)$. The well-known sum rule

$$\int_{-\infty}^{+\infty} d\omega f(\omega)A(\mathbf{k},\omega) = n(\mathbf{k}), \tag{2}$$

directly relates the energy-integrated ARPES intensity to the momentum distribution $n(\mathbf{k})$. Somewhat surprisingly, its usefulness has never been exploited in the ARPES literature.

We next focus on the Fermi surface $\mathbf{k} = \mathbf{k}_F$ and make a weak particle-hole symmetry assumption: $A(\mathbf{k}_F,-\omega) = A(\mathbf{k}_F,\omega)$ which is required to hold only for low ω (specifically, for the low frequencies at which there is significant T-dependence in the spectral function). It then follows that [5] $\partial n(\mathbf{k}_F)/\partial T = 0$, i.e., the area under the EDCs at $\mathbf{k}_F$ is independent of temperature. This is very clearly seen in the APRES data on Bi2212: the spectra themselves are very strongly T-dependent, but the integrated intensity remains constant; see Figs. 1 and 2 in ref. [5]. (Note that the weak p-h symmetry assumption made above does not determine the *value* of $n(\mathbf{k}_F)$ only its T-independence.)

We note that the observed sharpening of the ARPES peak in the superconducting state is *not* a "BCS pile up" in the density of states (a description frequently used in the literature). It is, in fact, a consequence of the above sum rule together with the dramatic decrease in the single-particle scattering rate (which determines the linewidth) below T_c. The very large linewidth, consistent with a non-Fermi liquid normal state, collapses to yield a resolution limited line at the lowest T, as the opening of the SC gap leads to a suppression of electron-electron scattering. This T-dependence is in qualitative agreement with analysis of optical and microwave data; a quantitative extraction of the frequency and temperature dependence

of the scattering rate from ARPES is an important open problem (which requires a better understanding of the ARPES "background").

We note in passing that the $n(\mathbf{k})$-sum rule can also be used to experimentally obtain the momentum distribution by energy integrating the ARPES spectra [5]. Quantitative studies of $n(\mathbf{k})$ will need an improved understanding of the ARPES "background", better momentum resolution, and theoretical input regarding the $\mathbf{k}$-dependence of the matrix elements.

3. Normal State of Bi2212

I will now briefly summarize the main results of a very detailed study of the electronic excitations in the normal state of Bi2212; see ref. [6] for details. As we shall see, the formalism established above will play an important role in interpreting the data both in the normal and in the SC state. All of the observed dispersing spectral features fall into one of three categories: (a) The main CuO band, with a Fermi surface area corresponding to 0.17 holes per Cu. (b) Umklapp bands which are simply $\pm\mathbf{Q}$ umklapps of the main band with $\mathbf{Q} = (0.21\pi, 0.21\pi)$ which corresponds to the superlattice (SL) distortion Q-vector along the b-direction. (In our notation $\Gamma\bar{M}$ is the $(1,0)$ direction, which is along the Cu-O bond, and ΓY is the $(1,1)$ direction). (c) There is some evidence for the "shadow bands" observed first by Aebi *et al.*[7], which are (π,π) "foldbacks" of the main bands.

Further, a detailed polarization analysis was undertaken. In all of the previous studies [2] of Bi2212, there was an apparent violation of selection rules in the X quadrant. The point is that since ΓX and ΓY are mirror planes, and a Cu orbital of $d_{x^2-y^2}$ symmetry is odd under reflection in these mirror planes, one expects a dipole-allowed transition when the incident photon polarization $\mathbf{A}$ is perpendicular to the mirror plane, but no emission in the "even"-geometry with the polarization parallel to the mirror plane. While this selection rule is obeyed along ΓY it is violated along ΓX. Clearly this "forbidden" $\Gamma X||$ emission cannot come from the main CuO band, but as shown in ref. [6] it originates from the SL bands which have an even combination that can account for it. We will return to the $\Gamma X||$ emission in the superconducting state below.

Another important conclusion is that only one Fermi surface (FS), enclosing the Y point,

is seen in the ARPES data (by this we really mean two degenerate Fermi surfaces which cannot be resolved). A FS is established by studying rapid variations of the integrated intensity, i.e., a peak in $|\nabla_{\mathbf{k}} n(\mathbf{k})|$. No evidence is found for a second FS enclosing the Γ point. The single FS crossing point along $\Gamma\bar{M}$, earlier thought to provide evidence for such a second sheet, is actually part of a superlattice band, as established by the polarization analysis in ref. [6].

On very general grounds, one expects that the two CuO_2 layers in a unit cell of Bi2212 should hybridize to produce a bonding and an antibonding band. However, it should be emphasized that two resolvable Fermi surfaces are *not* necessarily expected. Whether or not the two Fermi surfaces are resolvable depends sensitively on the exact doping levels and on the presence of Bi-O pockets, which are neither treated accurately in the theory nor observed in the ARPES data. However, there *is* a clear prediction from band theory: at $\bar{M}$, where both bands are below E_F, the bilayer splitting is the largest, of order 0.25 eV. Such a splitting should be observable (below T_c) even if there was a moderately large many-body renormalization.

The normal state spectrum at $\bar{M}$ is very broad because of many-body effects, and it could easily hide the two bilayer split bands. But, as discussed above, the spectrum acquires a sharp resolution limited quasiparticle peak deep in the SC state, and thus one should be readily able to see the bilayer splitting below T_c, if it exists. The question then is how to interpret the low temperature spectrum at $\bar{M}$ which consists of a sharp quasiparticle peak at about 25 meV and a broad bump at 100 meV, with a dip separating the two; see Fig. 2 in ref. [5] and Fig. 3 in ref. [6]. We must now choose between two hypotheses: (A) The dip and bump features arise due to many-body effects in a single spectral function $A(\mathbf{k},\omega)$, where the ARPES intensity is given by eqn. (1). (B) The bump is the second band which is resolved below T_c once the first band becomes sharp. The ARPES intensity in this case would be the a sum of two pieces each of which have the same form as in eqn. (1).

By changing the incident photon direction, and thus $\mathbf{A}$, we directly affect the dipole matrix element. Since there is only one matrix element involved in case (A), upon proper

rescaling both spectral features in the EDCs should match as **A** is varied. However, for case (B) there are two independent matrix elements which should vary differently with **A**, and thus if the EDCs are scaled so that one of the spectral peaks match, the other should differ significantly. By using this polarization dependence, Ding *et al.*showed that for Bi2212 hypothesis (A) is valid and the dip and two peaks are all part of a single spectral function. We note that a natural many-body explanation of the dip has been proposed [8] which leads to a suppression of the linewidth for $\omega < 3\Delta$.

The absence of any observable splitting within a bilayer is indeed quite remarkable and puts a much stronger constraint than incoherent c-axis transport from one bilayer to another. It should be noted that absence of bilayer splitting had been predicted by P. W. Anderson early on. It points to rather nontrivial many-body effects within a single plane. Consider the much simpler case of a two level system coupled to a bath: under certain circumstances it is known that the bath can destroy the coherent oscillations between the two levels, which would be the analog of interaction effects within the layers destroying the bilayer splitting.

4. Gap Anisotropy in Bi2212

I finally turn to the very important question of gap anisotropy in Bi2212. The discussion will be very brief because this topic has been discussed at length in refs. [9, 10, 11]. A detailed study of the gap in the SC state along the FS was undertaken in ref. [9]. Previous studies of the gap had used the qualitative criterion of a shift in the leading edge of the spectrum. The Argonne group made the first effort to model the data in terms of a spectral function and to extract quantitative gap estimates; see Figs. 2,3 and 4 in ref. [9]. While this procedure is quite unambiguous when dealing with the large gaps near the $\bar{M}$ point, the analysis of the small gap region is made difficult by uncertainties in modeling the lineshape and the background . Nevertheless, even after the sizable error bars on the gap estimates are taken into account, the first analysis of the X-quadrant data in ref. [9] suggested an extended-s-wave gap (see ref. [10]). But it was soon realized that, while the measured gap in the X-quadrant indeed shows two nodes, this result is due to the superlattice (SL) as discussed in detail in the erratum to ref. [9] and ref. [11]. The polarization analysis

described above, was used to prove that the small maximum, or hump, in the gap along ΓX was not on the main CuO band but rather on the even SL band (since the hump was observed in the $\Gamma X||$ geometry). In the Y-quadrant the Fermi surfaces of the main and SL umklapp bands are widely separated and thus the intrinsic gap should be readily observable. The presently available data in the Y-quadrant is less detailed than would be required to settle the gap controversy unambiguously. All that one can clearly say is that there is a region of about $\pm 10°$ about the diagonal (ΓY) where the gap is quite small; only further experiments will decide whether there is one node, or more, in this region.

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