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TITLE COMMENTS ON PHOTOELECTRON SPECTROSCOPY OF HIGH-Tc's

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Summary

"Comments on Photoelectron Spectroscopy of High-Tc's"

A.J. Arko

The photoemission discussion session during the Argonne conference on Fermiology of High-Tc's provided a forum to air a number of unresolved issues in photoelectron spectroscopy. These are: a) what is the exact energy dependence of the line width of the quasiparticle peaks ; b) are there any chemical potential shifts with hole doping; c) why is a superconducting gap not observed in Y-123; and d) different groups report different results in the band structure of Bi-2212.

The first issue, while much discussed, essentially becomes a non-issue in the sense that nearly all theories predict a linear as well as a quadratic energy dependence to the quasiparticle lifetime. Furthermore, the data are not yet good enough to distinguish between linear and quadratic dependence in the important region within 0.1 eV of E_F . Regarding chemical potential shifts, they very definitely are observed with hole doping both in Y-123 and Bi-2212 in spite of the claims by RVB enthusiasts to the contrary. In Y-123 the shifts are as large as 0.75 eV. The non-observation of a gap in Y-123 is puzzling, but may be related to surface reconstruction and an overdoped situation. The important question of whether we have one or two bands near E_F in Bi-2212 revolves around the surface quality of the samples studied by different groups. It is difficult to compare data taken at room temperature vs. data taken at low temperature when no documentation exists that a reconstruction did not occur. We suspect that the small second band championed by the Sendai group is a surface impurity band.

Comments on Photoelectron Spectroscopy of High-Tc's

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From the sessions on photoemission spectroscopy it is clear that numerous experimental questions pertaining to photoemission spectra remain unresolved in high-Tc research. Many of them are of crucial importance in piecing together the theoretical puzzle of this group of materials. I will try to enumerate only some of them which strike me as important, and point out where future research might be fruitful. Let's consider them in detail, and hope that they spark some discussion.

1. Line width of the quasiparticle peaks

Although Dr. Petroff has talked about this at some length, I would like to re-emphasise the importance of these measurements. A number of theorists have used the apparent linear dependence of the linewidth relative to E_F as conclusive proof of their favorite theory. However, as Dr. Petroff pointed out, such linear behavior may be endemic in the periodic table. Actually, researchers have simply not looked carefully enough to determine how the linewidth variation goes in normal materials, those in which there is no question about the Fermi liquid nature of the quasiparticles. There has not been a compelling reason to do so up till now, nor was the experimental resolution sufficient to allow it. It appears, however, that many Fermi liquid theories also predict a linear dependence of peak widths with energy over a limited range of energies. I believe that careful measurements in normal metals, particularly two-dimensional Fermi liquids such as NbSe₂, would go a long way toward clearing up the present confusion.

In addition, it appears that there is some disagreement over how well the data fits a linear energy dependence. Dr. Jim Allen claims that one cannot distinguish between a linear and a quadratic fit. The data are simply not yet good enough even though they are the highest quality angle resolved data to date.

2. Spectral Changes With Doping

There are many questions remaining regarding the development of the metallic state from the parent Mott insulators. Clearly we are not dealing with rigid band shifts. One school of thought is that there is very little difference in the electronic structure of the insulators vs. the metals, and that the intensity at the Fermi energy develops via a Kondo-like interaction with the conduction bands which increases with doping. In this variation of the Anderson model there is no chemical potential shift at all with doping. Some of the doping experiments of Veal et al. would at first glance seem to support such a conclusion since, after all, the Fermi surface (at least the part associated with the plane band) seems invariant even for doping levels which do not support superconductivity. This latter is actually a remarkable and confusing result.

But let us look at some other facts. In the first place, the band associated with the chains appears to be missing in the low-doped 123's. Secondly, chemical potential shifts (small, to be sure) have been observed in the 2212 structure with small oxygen doping. Thirdly, our early data have shown that there is a significant decrease (perhaps as much as 20%) in the overall width of the valence bands between the metallic and the insulating state. Finally the observation of the phenomenal, strongly dispersive, -1 eV peak seems to depend crucially on doping. Thus it would seem that there are substantial changes in the overall electronic structure between the insulators and the metals. Perhaps one can invoke a phase transition between the insulating and the metallic state. Within this picture the Fermi surface exists locally even at small doping (but not the chain band) and grows in intensity at greater oxygen stoichiometries. The chain band develops only at higher concentrations.

3. The Superconducting Gap

The new field of research, i.e., a study of the superconducting gap via photoemission, has opened up interesting new possibilities. It is now possible to study gap anisotropy on a microscopic scale, study surface superconductivity, as well as directly study the density of states in the superconducting state.

With regard to the superconducting density of states, there is complete agreement that the large pile-up just below E_F is BCS-like. However, there is additional structure at about -0.09 eV, which occurs first at T_c and grows with decreasing temperature, and for which there is little agreement. The Stanford group, which first reported this feature, now reports substantial anisotropy for this feature. This would seem to rule against the marginal Fermi liquid theory explanation which predicts no anisotropy for this feature. The idea of interplanar coupling resulting suddenly in three-dimensional bands at T_c also seems tenuous in view of the existence of the feature over such a wide range of k -values. To a much smaller degree it may exist in all parts of the zone.

The anisotropy of the gap itself is also being brought into question. Initial reports by Olson et al. indicated an isotropic gap within the basal plane. The Stanford group, however, claims to find nearly a factor of two anisotropy within the basal plane, which seems to scale with the -0.09 eV feature. The discrepancies may be traced to sample differences. However, if the anisotropy of both the gap and the -0.09 eV feature proves correct, then the two are marching in step and it may behoove us to look more carefully at Bosonic mechanisms for superconductivity, and possibly interpret the -0.09 eV feature as a manifestation of α^2F .

4. Band Structure of Bi-2212

In general there is reasonable agreement between various groups regarding the electronic structure of Bi-2212. There is, however, one major point of disagreement. This has to do with the number of bands crossing E_F . The Ames and Stanford groups report a single band with some complications around the M-point, while the Sendai group reports two bands. To complicate the matter further, Manzke et al. report a single band but different from the American groups, and equal to the smaller of the Sendai bands.

Since I was involved in the work of both American groups, I can report that the smaller band was actually observed, but only at 18 eV photon energy where there is a substantial enhancement, possibly due to the oxygen resonance. The intensity of this band was very small at other photon energies, and furthermore seemed to scale inversely with the quality of the cleaved surface, while the principal plane band intensity scaled directly with surface quality. This casts some doubt on the intrinsic nature of the smaller band, but obviously does not rule it out. As further evidence of our observations, in our initial attempts at photoemission in Bi-2212, our samples were baked at $\approx 150^\circ\text{C}$ along with the rest of the vacuum system in order to obtain a good vacuum. We discovered that this resulted in some sample deterioration so that even specimens cleaved at low temperatures failed to show the principal plane band, but they did show the smaller, or Manzke band. With this as evidence, we would certainly suspect specimen damage in any sample which fails to show the principal plane band. Whether this evidence is sufficient to rule out the smaller band as being intrinsic is still open to question, but it certainly is suggestive.

The resolution of this point is of some importance since several theories of high- T_c 's depend on the existence of the two bands or pieces of the Fermi surface. It is all the more urgent since there are clearly multiple pieces of Fermi surface in well oxygenated 123. On the other hand, lower oxygen stoichiometries apparently display a single piece of Fermi surface even though the sample is still superconducting.

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