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Photoemission from the High T_c Superconductors

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The electronic structures of $YBa_2Cu_3O_x$ and $YBa_2Cu_4O_8$ were studied by angle-resolved photoemission with an energy resolution of better than 10 meV. A detailed study in the 1st and 2nd Brillouin zone of untwinned single crystals shows the presence of "extended" saddle point singularities in the band structure in the vicinity of the Fermi energy, which give rise to van Hove singularities in the density of states. The binding energy of the singularity depends on the doping. We show that this extended saddle point singularity leads to a density of states which diverges as $\epsilon^{-1/2}$, which in turn can lead to very high transition temperatures even in a BCS scheme with weak coupling.

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Angle-resolved photoemission spectroscopy (ARPES) is an ideal tool for the study of the electronic structure of the high temperature superconductors (HTSC's), as it allows the determination of both the energy and momentum of electrons in the solid. Here we show how this capability is used to determine the energy spectrum in $YBa_2Cu_3O_{6.9}$ (Y123) and $YBa_2Cu_4O_8$ (Y124). Furthermore, we show that the nature of the energy spectrum of the CuO_2 planes near the Fermi energy (E_F) exhibits a new kind of van Hove singularity with profound consequences for high temperature superconductivity. Fig. 1a shows a typical photoemission energy distribution curve from an untwinned syngle crystal of Y124 covering a wide energy range (All of the data presented here were taken on untwinned single-crystals with polarization of the photon beam in the $\Gamma - Y$ plane, along the $\vec{b}$ axis of the crystal). The valence band extends from E_F to approximately 6 eV below E_F. The intensitty below the bottom of the valence band is mostly due to inelastically scattered electrons. Sharp peaks corresponding to particular inital states can be seen in the vicinity of E_F. The intensity of these peaks is very sensitive to the matrix elements governing the transition from intial to final states, as can be seen by comparing Figs. 1a and 1b. Both represent the energy distribution curves (EDC's) of elec-

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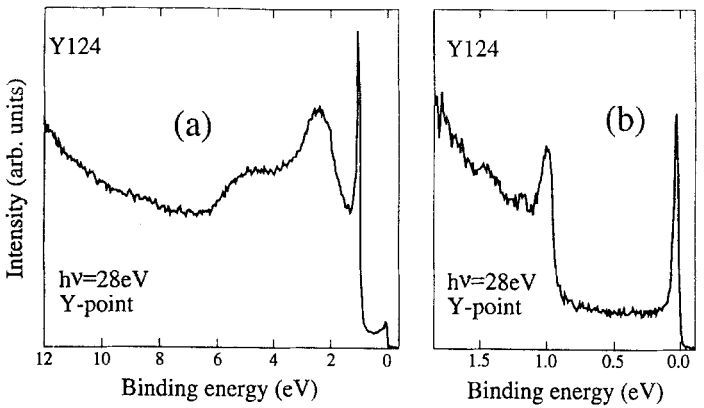

Fig. 1. a) EDC from Y124 at the Y symmetry point obtained with a photon energy of 24 eV; b) same as a), but with photon energy 28 eV.

trons originating at the Y symmetry point, the only difference being a 4 eV change in photon energy. However, one can see that the peaks near E_F have reversed intensities, indicating strong matrix element effects.

States far away from E_F are not relevant to superconductivity, therefore we will concentrate on the prominent peak observed just below E_F. Fig. 2a shows the EDC's obtained along the $\Gamma - Y$ symmetry line in the first and second Brillouin zones (BZ's) in Y124. It can be seen that a band disperses towards the E_F but does not cross it, remaining instead at a very small binding energy of 19 meV. The peak remains very close to E_F for a large portion of the BZ. The right panel in Fig. 2b shows the same peak near E_F. Now the energy scale is expanded by one and a half orders of magnitude (it is in milli-electron volts), and the peak is dispersing along the Y to S direction, the direction perpendicular to that in Fig. 2a.

This behavior constitutes a saddle point, where the energy spectrum has a maximum along one direction of momentum, and a minimum along the perpendicular direction. Furthermore, our systematic studies show that near the Y point, this peak has little dispersion in the k_z direction, as one expects from a two-dimensional system. Some of the data has already been published[1] and is not reproduced here. The position of this peak depends on the level of doping. It is observed in Y123 much closer to E_F, at a binding energy of less than 10 meV, as shown in Fig. 3a. We have drawn a curve through the peaks to indicate their position as a function of momentum.

In Y123 this feature persists for all doping levels for which the sample is superconducting. Fig. 3b shows the EDC's obtained in the vicinity of the Y point, both along the $\Gamma - Y$ and $Y - S$ symmetry directions. Based on this evidence, and by comparison with first-principles photoemission calculations,[2] we conclude that this feature originates in, and is intrinsic to, the electronic structure of the CuO_2 planes. The results are summarized in Fig. 4, which show the experimental band structure, $\epsilon(\vec{\mathbf{k}})$, of the feature as a function of momentum along the $\Gamma - Y$ and $Y - S$ symmetry lines. It can be seen that the feature exhibits an extended maximum along the $\Gamma - Y$ direction, while it exhibits a minimum along the $Y - S$ direction.

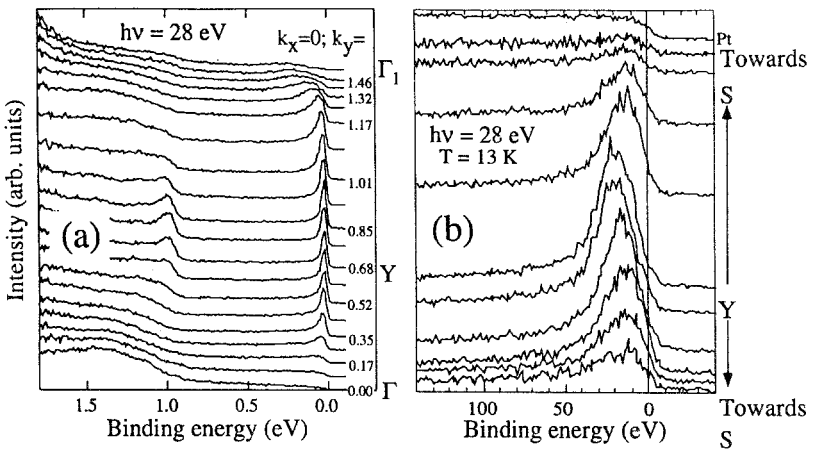

Fig. 2. (a) EDC's along the $\Gamma - Y$ symmetry line in Y124; (b) Dispersion of the peak shown in (a) but along the $Y-$S symmetry line, the symmetry line perpendicular to the one in (a).

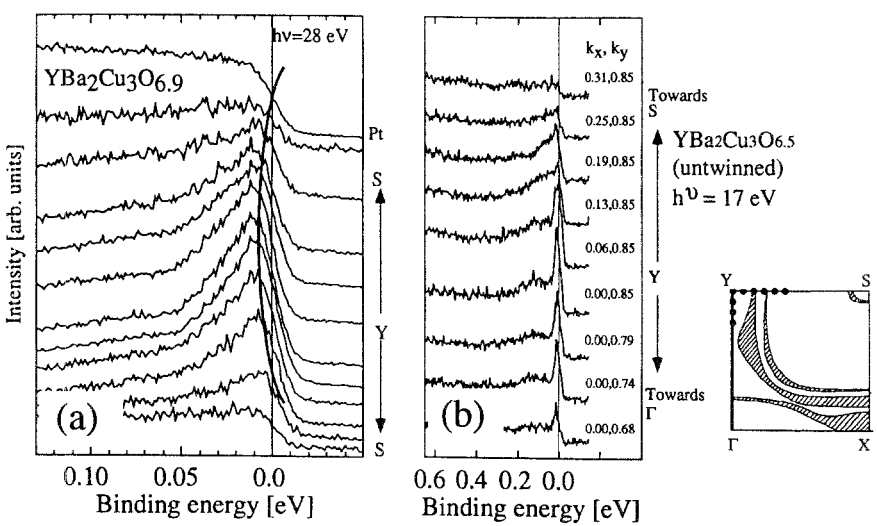

Fig. 3. (a) EDC's along the $Y - S$ symmetry line in Y123. The peak is now much closer to E_F compared to Y124; (b) EDC's obtained around the Y point in untwinned $YBa_2Cu_3O_6.5$. The peak at E_F remains as the doping decreases. The diagram on the left shows the points on the BZ where the data was obtained.

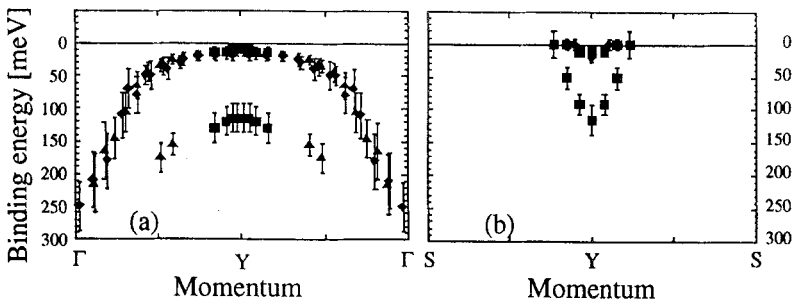

Fig. 4. a) Experimental band structure along a) the $\Gamma - Y$ and b) the $Y - S$ symmetry lines.

This "extended" saddle point in the band dispersion constitutes, by definition,[3] a van Hove singularity. It was pointed out by Andersen, et al.[4] that Y123 should exhibit a saddle point singularity which is bifurcated along the $\Gamma - Y$ direction. Experimentally, we find that the bifurcation has resulted in an "extended" saddle point, shown in the surface plot in Fig. 5.

Many mechanisms were proposed to explain the high T_c 's in cuprate superconductors, including the presence of a van Hove singularity near the Fermi energy. This proposal arose even before the discovery of the HTSC's, when Scalapino and Hirsh[5] showed that the presence of a logarithmic singularity near the Fermi energy changes the energy scale from that of phonons to that of electrons, $T_c \simeq E_F \exp(-1/\lambda^{1/2})$, leading to high T_c's. Once the HTSC's were discovered, Friedel[6] suggested that this mechanism might indeed apply in these materials. So far, there has only been indirect evidence for a singularity in the electronic density of states near E_F, such as the discontinuity of the specific heat capacity at T_c, the isotope effect and the quasiparticle lifetime broadening.[7,8] Here we find an "extended" saddle point singularity in the electronic band structure. The extended nature of the singularity is most significant, as it *qualitatively* changes the nature of the divergence in the density of states.[9] This peak had been observed before by Manzke, et al.[10] and Tobin, et al.,[11] although they did not determine that it constitutes a saddle point in the band structure. Our ARPES measurements show that not only is there a saddle point in the band dispersion, but that its extended character causes the dominant factor in the DOS to diverge not as a logarithm, but as a much stronger $\epsilon^{-1/2}$.[9] In this case, if one assumes a BCS mechanism, T_c scales as[9]

$$T_c = (1.346)^2 \frac{g^2 2 m_x k_{y_0}^2}{(2\pi^4 d^2} \sim E\lambda_0^2 \qquad (1)$$

If $E \sim$ 1eV and $T_c \sim$ 100 K, (1) yields the usually normalized interaction constant λ_0 of the order of 0.1 -a rather small value. This means that the interaction can have any origin, including phonons, as the most probable cause.

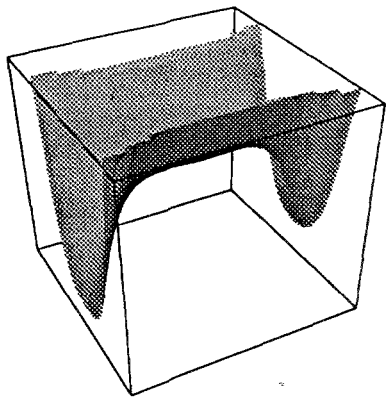

Fig. 5. Three-dimensional plot of the experimental energy spectrum showing the "extended" saddle point centered at the Y symmetry point.

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