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Evidence for a second one-dimensional set of states shedding light on the normal phase of high-T_c superconductors

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We have identified a set of electronic states with a one-dimensional dispersion in the $\Gamma=(0,0)$ to $M_1=(\pi,0)$ direction crossing the Fermi surface at one point $k_F=0.2\pm0.03\pi$ by angle-resolved photoemission. The one-dimensional character of these electronic states is demonstrated by missing dispersion along the orthogonal direction, observed in energy-distribution curves, and by k-space mapping of the Fermi surface, using angle scanning photoemission. The observed electronic states beyond the well-known large Fermi surface provoke the models based on charge and spin ordering in the CuO_2 plane of high-T_c superconductors. [S0163-1829(98)51218-0]

Over the last few years, experimental data have been accumulating showing that the normal state of high-T_c cuprate superconductors has similarities with other complex materials such as new colossal magnetoresistance compounds and isostructural nickelates.[1–9] It is becoming accepted that the anomalous electronic properties of these materials are typical of complex materials where charge, spin and lattice fluctuations play a key role for their theoretical understanding.[10–11] Angle resolved photoemission has been widely used to study the electronic properties of high-T_c superconductors.[12–18] A variety of unique features in the photoemission spectra including extended van Hove singularities,[12,13] opening of a pseudogap in underdoped samples,[14] shadow bands assigned to magnetic interactions,[15] and umklapp satellites[16] have been observed. A global view of the Fermi surface measured by angle scanning photoemission of an optimally doped system has shown the asymmetry of the large Fermi surface[18] that has been correlated with a one-dimensional (1D) charge segregation in diagonal stripes in the CuO_2 plane observed by anomalous x-ray diffraction.[19]

In the present paper we provide direct evidence for a one-dimensional set of states with total dispersion of $\Delta E=80$ meV, i.e., of the order of antiferromagnetic exchange interaction $J=125$ meV.[4] These electronic states with $k_F'\sim0.2\pi$, in units of $1/a$, where $a=3.8$ Å, in the Cu-O-Cu direction, might be correlated with the one-dimensional low-frequency incommensurate spin fluctuations with a wave vector $q_S\sim k_F'$ along the same direction reported by magnetic scattering studies.[4–6] The results may answer the frequently asked question of how the lattice distortions ordering observed along the (π,π) direction[19,20] could be reconciled with the 1D magnetic fluctuations along the $(\pi,0)$ direction.[4–6]

The angle-resolved photoemission (ARPES) measurements were carried out at the Laboratoire pour l'Utilisation du Rayonnement Electromagnetique (LURE) (Orsay, France) on the SU6 undulator beamline. A $Bi_2Sr_2CaCu_2O_{8+\delta}$ (Bi2212) crystal of size $6\times6\times1$ mm^3, grown by the floating zone method,[21] was used for the measurements. It has a stoichiometric 2212 composition doped by interstitial oxygens. We have characterized this monodomain crystal by x-ray synchrotron radiation diffraction showing sharp diffraction lines limited by resolution. It is at optimum doping giving the highest critical temperature for this family of cuprate superconductors, $T_c=91$ K with $\Delta T_c\sim1$ K. The same T_c is found for the bulk and for each cleaved surface as measured by surface resistivity using inductive coils. We have used the constant initial energy angle scanning photoemission[18,22] accompanied with the standard approach based on energy distribution curves, exploiting high intensity of the synchrotron radiation emitted by an undulator source. The experiments were performed in an ultrahigh vacuum (UHV) chamber (base pressure 7×10^{-11} mbar) equipped with an angle-resolving hemispherical analyzer and a high-precision manipulator permitting an azimuthal sample rotation (ϕ) of 360° and polar emission angle relative to the surface normal (θ) of 90°.[23] The angular resolution used for the Fermi surface mapping is 1.5° while for the energy distribution curves (EDC) is 1°. The spectrometer energy resolution was about ±50 meV. The measurements were performed using the linearly polarized synchrotron light with photon energy of 32 eV in the even symmetry. In this geometry, the polarization vector of the synchrotron light, the wave vector of the emitted photoelectron and the surface normal were in the same horizontal plane that plays the role of a mirror plane and the

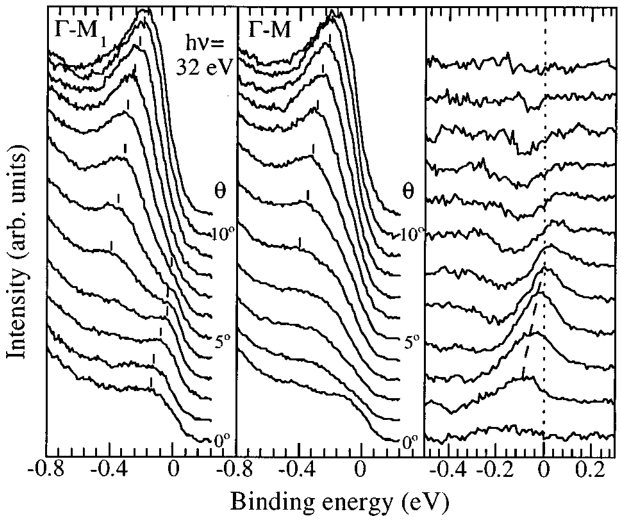

FIG. 1. Energy distribution curves (EDC) measured along the $\Gamma->M_1=(\pi,0)$ (left), the orthogonal $\Gamma->M=(0,\pi)$ direction (center), and the difference between the two (right). The 1D band appears in the $\Gamma->M_1(\pi,0)$ dispersing from -80 meV to E_F crossing at $k_F=(0.2\pi,0)$.

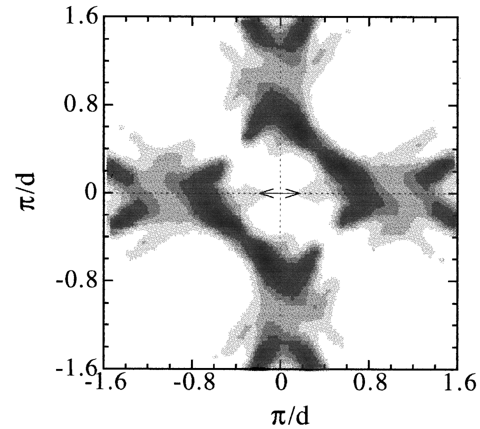

FIG. 2. Photointensity distribution of states near the Fermi surface obtained by constant initial-state angle scanning photoemission. The intensity above 15% of the maximum intensity is plotted to remove the low intensity features due to umklapp satellites. The intensity increases from light to dark in a grey scale. We have used the following notations; $\Gamma=(0,0)$, $M_1=(\pi,0)$, $M=(0,\pi)$, $X=(\pi,\pi)$, $Y=(-\pi,\pi)$, and $Y_1=(\pi,-\pi)$. The one-dimensional (1D) band can be clearly observed only in the $\Gamma=(0,0)->M_1=(\pi,0)$ direction crossing E_F at two points $(\pm 0.2\pi,0)$ indicated by the arrows.

transition from the initial states with even symmetry (Cu $3d_{x^2-y^2}$, O $2p_{x,y}$) is allowed.[12,16] This geometry has been used to have maximum emission intensity along the $(\pi,0)$ and $(0,\pi)$ directions. The data have been collected at 290 K. The sample was carefully aligned crystallographically by x-ray diffraction. It was cleaved in the UHV chamber and its alignment was ensured by low-energy electron diffraction. The flatness of the sample surface was controlled by laser reflection. The alignment of crystal with respect to theta and phi angles is confirmed by photoelectron diffraction of deep core levels.

The energy distribution curves (EDC's) measured along the $\Gamma-M_1(\pi,0)$ (left) and $\Gamma-M(0,\pi)$ (center) directions are shown in Fig. 1. The EDC's in the left panel of Fig. 1 have been collected with the photon polarization along $\Gamma-M_1$, while the photon polarization is along $\Gamma-M$ for the EDC in the central panel of Fig. 1. For this reason the transitions from initial states due to the CuO_2 layers are dipole allowed in both experimental curves, as can be seen directly by their similar strong intensity. There are dispersing features in both directions, however EDC's in the two directions show clear differences in their line shapes. The main spectral band is clearly visible in both directions for polar angles above 5° off the Γ point and disperses from -350 meV towards the Fermi level. It should be recalled that this main band in this direction does not cross the Fermi level and remains below it (~ 20 meV) giving an extended van Hove singularity.[12,13]

While the main band appears quite similar in the two orthogonal directions, the EDC's along $M_1=(\pi,0)$ shows a second dispersive spectral feature at lower angles with a smaller intensity. This second band crosses the Fermi level at around $k_F'=0.2\pi$ with a total energy dispersion $\Delta E \sim 80$ meV. On the other hand, we do not see this second band in the EDC's measured along the orthogonal $\Gamma-M=(0,\pi)$ direction. This second band can be clearly seen in the difference spectra plotted in Fig. 1 (right). This second band appearing only in one direction was reproducibly observed on different runs performed on different cleaved surfaces ascertaining its intrinsic nature. This result provides direct evidence for a new set of electronic states at the Fermi surface having one-dimensional character along the Cu-O-Cu direction.

The first indication of this second set of states was provided by our earlier paper[18] where the topology of the Fermi surface was obtained by constant initial-state angle scanning technique. We have confirmed the presence of the one-dimensional states only near the Fermi surface by further experiments and they are indicated by arrows in Fig. 2 which shows the photointensity distribution above the 15% level of the maximum. The gray scale represents intensity of the emitted photoelectrons excited from the initial state having constant energy E_F and in-plane wave vector ($k_{\parallel}$) spanned over reciprocal space of the two-dimensional CuO_2 plane. This figure shows the envelope of equipotential lines of the band structure within the experimental energy resolution near the Fermi level. The Fermi surface shows clear difference between the $\Gamma-M=(0,\pi)$ and $\Gamma-M_1=(\pi,0)$ directions with a presence of the one-dimensional band, indicated by the arrow, that can be evidently seen only along the $\Gamma-M_1=(\pi,0)$ direction as photointensity spots around $k_F'=\pm 0.2\pi$ $(\pm 0.03\pi)$.

To further ascertain this we have measured photointensity at the Fermi surface by scanning the polar angle along the $M_1=(\pi,0)$ and $M=(0,\pi)$ directions across Γ point. The polar scans along the two directions are shown in Fig. 3. The photon polarization is along $\Gamma-M_1$ for the angle scanning in the $\Gamma-M_1$ direction (dashed line), while it is along $\Gamma-M$ for the angle scanning in the $\Gamma-M$ direction (solid line), therefore the transitions from initial states due to the CuO layers are dipole allowed in both experimental curves. The two curves are practically identical in the range between 0.35π and π while an additional contribution appears in the low-k range 0–0.25π only along the $\Gamma-M_1=(\pi,0)$ direc-

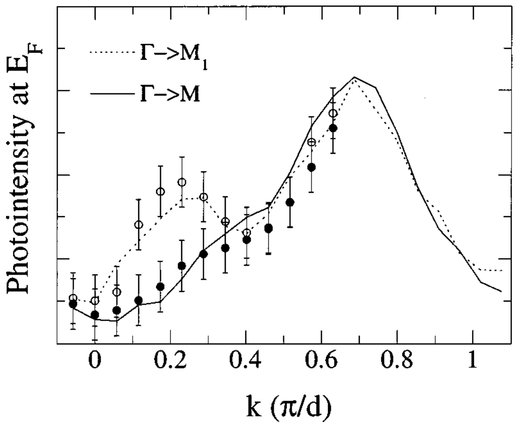

FIG. 3. The polar scans of the photointensity at the Fermi level along the $\Gamma->M$ (solid line) and $\Gamma->M_1$ (dotted line) directions. The crossing of the 1D band at the Fermi surface is clearly visible by a peaked structure in the polar scan along the $\Gamma->M_1$ direction at 0.2π and it is missing in the other direction. The unklapp satellites give weak shoulders at $\sim 0.30\pi$ along the two directions and is clearly visible as a shoulder in the polar scan along the $\Gamma-M$ direction. The data points represent the photointensity at the Fermi surface obtained from the EDC's (Fig. 1) along $\Gamma->M$ (closed circles) and $\Gamma->M_1$ (open circles).

tion. This contribution is due to the 1D band that gives a peaked structure in the vicinity of $k_F \sim (0.2\pi,0)$ corresponding to its Fermi level crossing. On the other hand we could see only a diffused photointensity peaking around 0.32–0.4 π in the $\Gamma-M$ direction that is expected due to umklapp process of emitted photoelectrons by the modulation of the BiO plane. Our results in the $\Gamma-M$ direction are in perfect agreement with the data of Randeira *et al.*[16] where by assuming a simplified tetragonal symmetry there is no distinction between $\Gamma-M$ versus $\Gamma-M_1$ directions. The crossing at $(0.2\pi,0)$ observed in the present work only in the $\Gamma-M_1$ direction can be clearly distinguished from the above-mentioned umklapp reflections that are weaker and are present in both directions. It is possible that the disorder, due to nonstoichiometry of metallic elements in the samples, has masked the breaking of the symmetry between the two directions in previous studies. We have used a photon energy of 32 eV since we have higher photon flux at this energy, however no variations were observed using the standard energy of 25 eV, and the anisotropy of the new 1D band shown in Fig. 1 between the $\Gamma-M$ and $\Gamma-M_1$ directions is clearly an intrinsic effect independent on the used photon energy.

To summarize the experimental findings the joint analysis of energy distribution curves and angle scanning data on a perfect crystal at optimum doping has allowed us to clearly identify a set of states with 1D character. We have plotted in

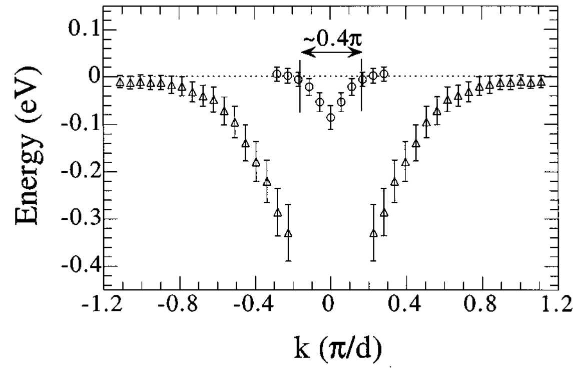

FIG. 4. Dispersion in the $\Gamma->M_1$ direction of the second set of 1D states identified in this work and of the main band.

Fig. 4 the dispersion of this set of states having one-dimensional character forming a narrow band ($\sim$80 meV) and small k_F' ($\sim 0.2\pi$) along the $(\pi,0)$ direction of the Brillouin zone. For this one-dimensional band we expect charge fluctuations with the nesting wave vector $\mathbf{q}_c = 2\mathbf{k}_F'$ ($\sim 0.4\pi$) as shown in the figure.

The 1D incommensurate low-frequency spin fluctuations with wave vector $\mathbf{q}_s \sim (0.2\pi,0)$ observed in inelastic neutron scattering in cuprate superconductors[4–6] are expected to be associated with charge fluctuations of wave vector $2\mathbf{q}_s$ that is similar to the measured nesting vector $\mathbf{q}_c$. Therefore we argue that this one-dimensional band is related with the 1D spin fluctuations.[4–6] This corresponds to an instantaneous spin modulation with a period of about 9–10 Cu sites in the Cu-O-Cu direction. On the other hand x-ray anomalous diffraction and extended x-ray absorption fine structure (EXAFS) have been jointly exploited to derive the stripe structure in the CuO_2 lattice. The lattice modulation in the CuO_2 is found to be along at 45° from the Cu-O-Cu direction, with wave vector $(\sim 0.2\pi, \sim 0.2\pi)$ direction in Bi2212 forming a superlattice of quantum stripes.[9,18–20] The breaking of the symmetry between the $(\pi,0)$ and $(0,\pi)$ directions is assigned to the tilting of the CuO_4 square planes in the LTT stripes only in one direction.[9,20] Therefore in our opinion the presence of a second set of 1D electronic states in the present ARPES data is correlated with spin fluctuations along the vertical direction that coexists with diagonal stripes of distorted lattice, and it supports the scenario of the T_c amplification by an 1D ''shape resonance'' effect.[24]

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