Unusual electronic ground state of a prototype cuprate: band splitting of single CuO$_2$-plane Bi$_2$Sr$_{2-x}$La$_x$CuO$_{6+\delta}$

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The momentum dependence of the split band of Bi$_2$Sr$_{1.6}$La$_{0.4}$CuO$_{6+\delta}$ is investigated by very highly resolved photoemission along the ΓM-line. Since bi-layer effects can not be present in this single-layer material the results have to be discussed in the context of one-particle removal spectral functions. The most prominent are microscopic phase separation including striped phase formation, critical fluctuations coupled to electrons (hot spots) or even spin charge separation within the Luttinger liquid picture, all leading to non-Fermi liquid like behavior in the normal state and having severe consequences on the way the superconducting state forms.

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The determination of the k-resolved spectral function is a key issue for a deeper understanding of the cuprate superconductors, since even the non-superconducting ground state poses severe theoretical challenges for a description within some strongly correlated, non-Fermi liquid model. The advance achieved over the last years in higher resolved photoemission as input for these theories is impressive, but unfortunately to a very great extent focussed on Bi$_2$Sr$_2$CaCu$_2$O$_8$, the Bi-cuprate with two CuO$_2$-planes per unit cell, where bi-layer splittings are expected to influence the photoemission lineshape. Therefore, measurements on prototype single CuO$_2$-layer materials like Bi$_2$Sr$_{2-x}$La$_x$CuO$_{6+\delta}$ with sufficiently decoupled layers are in high demand to investigate the characteristics of a single CuO$_2$ layer slightly above $T_C$ of 29 K with minimum temperature broadening of the spectra. By resistivity measurements on this compound down to zero Kelvin in high magnetic fields it could be shown that, unlike some other cuprates strict confinement of the carriers to the CuO$_2$-planes occurs: it possesses metallic non-Fermi-liquid character in the planes and insulating character perpendicular to them, showing a ratio of up to $\rho_c/\rho_{ab} = 10^5$ at zero Kelvin. On the other hand the observation of two distinct emissions near the Fermi energy on Bi$_2$Sr$_{2-x}$La$_x$CuO$_{6+\delta}$ by in situ polarization dependent photoemission near the (π,0)-point by Manzke et al. has enormous consequences on the description of the ground state of cuprate superconductors. In this letter we will therefore further investigate the individual dispersions of these emissions for the n=1-layer Bi-cuprate at optimum doping and discuss the observed splittings within the framework of existing non-Fermi liquid theories.

For photoemission with 34 eV photon energy and in situ variation of polarization at BESSY in Berlin we used an experimental setup described previously. The energy resolution was 30 meV and the angle resolution ±1°. The data taken with 22 eV photon energy were obtained at the U-PGM beamline of the Synchrotron Radiation Center in Madison-Wisconsin (SRC) with a SCIENTA-SES200-analyzer with an overall energy resolution of 16 meV and the angle resolution ±0.18°. We present photoemission data from optimally doped Bi$_2$Sr$_{2-x}$La$_x$CuO$_{6+\delta}$ ($x=0.40$, $T_C=29$ K) single crystals. All measurements were performed slightly above the critical temperature (35 K at BESSY and 45K at SRC). The samples were rectangular shaped with the long side along the crystallographic a-axis, confirmed by Laue-diffraction, and have a typical size of 5x2 mm$^2$. The growth of the single crystals has been described previously.

FIG. 1 gives a direct indication of the splitting of the Zhang Rice singlet state band by different methods. In the upper panel the separation of two distinct emissions at the (π,0)-point of the Brillouin zone is demonstrated by applying different polarization geometries. Both spectra were taken without moving the analyzer or the sample in succession within one hour. The polarization change was solely achieved by tuning the crossed undulator beamline. Following this procedure allowed the same sample spot to be measured as well as eliminating potential uncertainties due to sample misalignment. Although both polarization geometries, described in the figure caption of FIG. 1 are identical with respect to dipole matrix element selection rules, large differences in the intensity close to $E_F$ occur. Since the spectra are absolutely normalized to photon flux the almost vanishing polarization dependence of the emission at higher binding energy (labelled H) is not an artefact. The polarization acts strongly at the second spectral contribution at $E_F$ (labelled S), almost switching it on and off. The difference spectrum therefore shows solely emission S, its halfwidth having the size of the total energy resolution of 30meV. This sharp emission S will be investigated further below. While the spectra in the upper panel were recorded with a relatively large angular resolution of ± 1°, requiring to work at the M-point where the dispersion of the bands is minimal, in the lower panel we show spectra taken at the SRC with an angular resolution of ± 0.18° and an energy resolution of 16 meV enabling a detection of the dispersion of the states. Applied is a geometry in which
both emissions, S and H, are excited. One sees clearly
the dispersion of two individual emissions approaching to
a structure not resolvable into individual contributions
near the M-point. Additional spectra at higher angles (not shown) showed an symmetric reappearance of
the two individual structures around the M-Point. Also
at higher photon energy (32eV) two individual contribu-
tions were observable.

In FIG. 2 a selection of spectra along the Γ-M direction
from FIG. 1 is shown together with a fit of the spectral lines contributing to the spectra. The spectra were mod-
elled by two Lorentzians convoluted with a Gaussian of
width for the experimental resolution and cut off by a Fermi-Dirac distribution. The background,
although relatively weak in the spectra series, was only
modelled by the Shirley background 8. Thus, for some
spectra it was found necessary to set a limit to the fit
region relatively close to the peak at higher binding en-
dergy due to its asymmetric shape. This emission line
H at higher binding energies has a larger halfwidth and
stronger dispersion relative to the low energy line S. The
fit yielded typically an intrinsic width of 13 meV for emis-
sion S and 51 meV for emission H around the M-point.
Both are found to be separable by the fit even at the M-
point. The splitting has been verified on a total of three
samples.  

FIG. 1. Upper panel: Normal state (T = 35 K) photoemis-
sion spectra of optimally doped Bi$_2$Sr$_{2-x}$La$_x$Cu$_2$O$_{6+δ}$ at
the M-point for two polarization geometries as shown in the
inset (hν=34eV). In this experiment the sample position was
fixed and the vector potential of the synchrotron radiation
was switched by 90°. Drawn line: E ⊥ ΓX; broken line: E∥ΓX
; points: difference spectra.
Lower panel: Spectra series (T=45K) along a part of the ΓM-
direction as indicated in the inset as thick black line with the
polarization in the detection plane (hν=22eV).

FIG. 2. Selection of normal state (T = 45 K) photoemission
spectra of FIG. 1. The fit is described in the text. The
shortcoming of the fit towards the higher binding energy tail
of the spectra is a result of the asymmetry associated with
the higher binding energy peak which was not considered in
our simple model calculation.
The spectra series along the Γ-Y direction in FIG. 3 shows the dispersion of the uppermost band in the Fermi surface region between the diffraction replicas due to the incommensurate (1x5)-superstructure (not shown). Unlike for the Γ-M-direction a clear separation into two individual contributions is not obvious at any of these spectra. As a test these EDC spectra were tentatively fitted similarly as before with two Lorentzians. One obtains two structures that do not merge at the Fermi energy crossing point. The dispersion of the low binding energy feature can be traced when crossing the Fermi energy. The high binding energy feature loses spectral weight upon approaching the Fermi energy and becomes very broad, making a definite statement whether it crosses $E_F$ or just approaches intimately very hard. One may conclude from this that unlike for the Γ-M direction essentially one asymmetric peak is present along ΓY.

FIG. 3. Normal state ($T = 45$ K) photoemission spectra in the EDC-mode (energy distribution curve) for optimally doped Bi$_2$Sr$_{2-x}$La$_x$CuO$_{6+δ}$ along ΓY. The polarization vector lies in the plane of the electron detection, the photon energy was 22 eV.

To arrive at a more quantitative understanding of the individual dispersions the fit results along Γ-M are shown in the dispersion curve of FIG. 4. The dispersion of the states can be traced continuously with respect to halfwidth and intensity. While the halfwidth of the low binding energy peak does not change significantly the higher binding energy peak sharpens considerably upon approaching M. If the dispersion of the lower binding energy feature is scaled by a factor of approximately 2.7 it coincides in dispersion with the higher binding energy feature.

FIG. 4. of states near $E_F$ as derived from FIG. 1

To attribute the observed splitting of the CuO$_2$-derived band unequivocally to an intrinsic origin, disturbing influences as resulting from the diffraction replicas or from possibly occurring BiO-pocket bands must be ruled out. In a detailed study Singh and Pickett calculated the near Fermi surface bands and the Fermi surface topology by a LAPW-method including spin-orbit effects for Bi-2201 with orthorombic distortion. They found five bands with origin from the BiO-plane forming small hole pockets around the M-points and one CuO$_2$-derived band forming a large Fermi-surface round the X(Y)-points. From our measurements along ΓM depicted in FIG. 1 and FIG. 2 no such $E_F$-crossing of BiO-bands is observed, which should be detectable with the high energy and angular resolution applied. This finding is similar to the situation for Bi-2212, where also no crossing of BiO-bands was reported in this direction. The other source of additional structures, namely diffraction replicas can be ruled out from three experimental observations: the two bands are degenerate on the entire, main Fermi-surface, they merge at temperatures exceeding 120 Kelvin and also for increased hole doping, which brings the system closer to the Fermi-liquid regime. These issues will be discussed in a forthcoming publication. The possibility of surface states can, most probably also be ruled out: these may be expected in more three-dimensional materials, preferably with broken bonds on the surface. Bi-2201 in contrast is extremely two-dimensional and cleaves between the weakly bonded BiO-layers. No surface reconstruction has been observed so far. Furthermore, the well studied Bi-
2212 is also known to be free of surface states.

In the case of Bi-2212 the dispersion of a single spectral feature near $E_F$ has been discussed with the marginal Fermi liquid model of Varma [10] or alternative approaches [11,12]. Another basic issue is the dimensionality of the system of interacting fermions in the CuO$_2$-planes. Anderson [13] has put forward the tomographic Luttinger model leading to Luttinger liquid behavior with spin and charge separation. In this context, Castellanì et al. [14] have investigated the low energy behavior of interacting fermions in continuous dimensions between one and two, discussing the possibility to obtain Luttinger liquid like behavior in this intermediate dimension.

The idea of spin and charge separation is also underlying the RVB-theory, first proposed by Anderson [13]. From photoemission-studies [16] it has been argued that the extended saddle point in ΓM-direction would render the band structure quasi-1D. Although the cuprates are structurally quasi two-dimensional there is increasing theoretical and experimental evidence that over a certain range of temperatures on a local scale stripe correlations make the electronic structure quasi-one dimensional [17]. Static or dynamic charge inhomogeneity has been found in several strongly correlated electronic systems and is not unique to the high temperature superconductors [17]. In the cuprates the formation of stripe correlations can be understood with the concept of frustrated phase separation [18].

The basic physics of spin charge separated, essentially one-dimensional electron liquids has been treated by Voit [19]. In the Luttinger liquid picture the dispersion of Voit’s models consisting of two singularities is described by only three parameters: the renormalized coupling constants $k_\nu$ ($\nu = \rho, \sigma$ for charge and spin) are the equivalent of the Landau parameters in the case of the Landau Fermi liquid. For spin rotation invariance [19] $k_\sigma$ is set to one i.e. this branch is essentially unrenormalized. With the velocities $v_\rho$ and $v_\sigma$ of the charge and spin fluctuations the scenario with $0 \leq k_\rho < 1$ and $v_\rho > v_\sigma$ describes repulsive and $k_\rho > 1$, $v_\sigma > v_\rho$ attractive interactions. Our measurements give support to a model with repulsive interactions ($k_\rho < 1$), generally assumed for HTc’s, since the dispersion of the holon is larger by a factor of 2.7 ($v_\rho > v_\sigma$). The experimental fact that the overall dispersion of the bands is smaller than obtained from single particle bandstructure calculations is possibly due to some complete renormalization of the electron system. One may think for instance of strong electron-phonon coupling. The experimentally observed band-splitting and different dispersions along the Γ-M-symmetry line of Bi-2201 can presumably not be mapped 1:1 onto this essentially one dimensional Luttinger model, but may find an explanation within an extention to a modified Luttinger model for the physical system under study. The different halfwidths of S and H can possibly be ascribed to a coupling of phonons to the charge but not to the spin degrees of freedom.

In the context of striped phase ordering Salkola et al. [20] studied the consequences of disordered charge stripes and antiphase spindomains for the properties of high temperature superconductors. The orientation of the stripes along the CuO-bonds (ΓM direction) leads to a situation, where the fourfold rotational symmetry of the ideal CuO$_2$-plane is broken through a plane at 45° to the CuO-bond. Reflection symmetry and the according selection rules are nevertheless obeyed for planes parallel and perpendicular to the stripes. In this view the slight orthorhombic distortion is not incorporated. If its effects are regarded as less important the polarization effects described in FIG. 1 and 2 may in parts be ascribable to this reduced symmetry. At present there is to our knowledge no theoretical study matching the present results perfectly. The theoretical investigation of a quasi one-dimensional HT$_C$ with stripes and its spectral function at the Fermi vector by Carlson et al. [21] shows a broad, incoherent peak above $T_C$, not in line with our measurements. This is possibly ascribable to the parameters used, which can of course greatly influence the line-shape. Also Seibold et al. [22] discussed the occurence of incommensurate CDW’s due to stripes but found a manifold of bands in the vicinity of $E_F$ also not corroborated by our measurements. Alternatively Caprara et al. [23] have studied the single-particle spectral properties of a model of coexisting antiferromagnetic and incommensurate charge-density-waves coupled to electrons in the context of the stripe-quantum-critical-point scenario. The deviations from Fermi-liquid behaviour were found near the points of the Fermi surface connected by characteristic wave vectors of the critical fluctuations, the so called hot spots. The interactions lead to a transfer of spectral weight from the quasiparticle peak to an incoherent peak. The spectra series calculated from this model along Γ-M showed however a larger separation of the two contributions than found in our experiment, possibly due to the parameters used.

In summary, we have observed the dispersion of two individual emissions with different velocities along the Γ-M direction for single-layer Bi-2201. The dispersion and halfwidth could be traced continuously. In line with polarization dependend measurements the halfwidth of the low binding energy emission is 13 meV around the M-point. Its singular and highly anisotropic character with respect to polarization is contrasted by the relatively broad (typ. 51meV), nearly polarization insensitive second emission at higher binding energy. Along the Γ-Y direction no clear splitting is observed. The observations were discussed in the context of current theories giving support to the idea of spin and charge separation, although no perfectly matching theory was found. When interpreted in the framework of exactly one-dimensional models a situation with repulsive interactions is obtained from a comparison to the experimentally observed disper-
I. ACKNOWLEDGEMENT

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