# Anomalies in the Fermi Surface and Band Dispersion of Quasi-One-Dimensional CuO Chains in the High-Temperature Superconductor $YBa_2Cu_4O_8$

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We have investigated the electronic states in quasi-one-dimensional CuO chains by microprobe angle resolved photoemission spectroscopy. We find that the quasiparticle Fermi surface consists of six disconnected segments, consistent with recent theoretical calculations that predict the formation of narrow, elongated Fermi surface pockets for coupled CuO chains. In addition, we find a strong renormalization effect with a significant kink structure in the band dispersion. The properties of this latter effect [energy scale ($\sim 40$ meV), temperature dependence, and behavior with Zn-doping] are identical to those of the bosonic mode observed in $CuO_2$ planes of high-temperature superconductors, indicating they have a common origin.

In one-dimensional (1D) systems, electrons are confined to motion along the atomic chains, making them strongly correlated [1]. The electronic properties of 1D CuO chains are especially interesting because they form the building blocks for $CuO_2$ planes, which display high-temperature superconductivity. The pairing mechanism in these systems is not well understood. One reason for this is the difficulty in the modeling of $CuO_2$ planes. A possible solution is to start with very weakly coupled CuO chains, which are well understood analytically, and then increase the coupling to a value typical for $CuO_2$ planes. Recently, a calculation [2] for coupled CuO chains was performed as a function of coupling strength using a variation of the dynamical mean field theory (ch-DMFT) [3–5]. It revealed the breakdown of a typical quasi-1D Fermi surface into narrow, elongated pockets that resemble the disconnected Fermi arcs observed by angle resolved photoemission spectroscopy (ARPES) in the pseudogap state of the cuprates [6]. This issue is very important as a number of recent experiments find quantum oscillations in $YBa_2Cu_3O_{7-\delta}$ (Y123) and $YBaCu_4O_8$ (Y124), which suggests the existence of very small Fermi pockets [7–10]. A detailed understanding of the physics of 1D CuO chains is also important because they provide an idealized model for stripes that are seen in some cuprates and which are thought by some to play a role in the mechanism of high-temperature superconductivity [11–15]. Surprisingly, the signature of magnetic fluctuations in stripes [16] very closely resembles that associated with the magnetic resonant mode seen in cuprates by inelastic neutron measurements [17]. Therefore the electronic properties of chains

may also provide important information about the relation between the magnetic resonant mode, high-temperature superconductivity, and stripes.

In this Letter, we use angle resolved photoemission spectroscopy and study the electronic properties of CuO chains in the high-temperature superconductor, $YBa_2Cu_4O_8$ (Y124). We observe a quasiparticle Fermi surface that consists of disconnected segments. This observation is in excellent agreement with, and directly confirms, the results of the ch-DMFT calculation for coupled chains [2]. The result raises the possibility that the quantum oscillations observed in Y123 and Y124 [7–10] occur in pockets due to CuO chains. Our data reveal the presence of a strong renormalization effect at an energy of $\sim 40$ meV and a small energy gap ($\sim 5$ meV) in the superconducting state. This effect is only observed along a small momentum region, where the Fermi surface of chains and planes cross, suggesting that it is caused by coherent hopping of electrons between the chains and planes. The renormalization effect disappears above $T_c$ and is almost completely suppressed in samples doped with only 1% of Zn. These properties and the energy scale ($\sim 40$ meV) are almost identical to those of the bosonic mode observed in superconducting $CuO_2$ planes [18–23], which suggests they have a common origin. Our data demonstrate that chains play a crucial role in establishing a 3D metallic state and superconductivity in Y-Ba-Cu-O at low temperatures [24,25].

Twin-free single crystals of underdoped pristine $YBa_2Cu_4O_8$ ($T_c = 80$ K) and 1% Zn-doped $YBa_2Cu_4O_8$ ($T_c = 60$ K), were grown by the self-flux method under

high oxygen pressure [26]. ARPES measurements were
performed at the PGM beam line at the Synchrotron
Radiation Center, USA, and at the SIS beam line of
Swiss Light Source, Switzerland. Both measurements
used a SES2002 hemispherical analyzer. The energy and
angular resolutions were 10–30 meV and ~0.15°,
respectively.

Figure 1(a) shows a typical band dispersion map from
the CuO chains. A schematic diagram of the chain domains
at the sample surface is shown in the inset of Fig. 1(b). As
we reported in a previous paper [27], two bands originating
from CuO chains are clearly seen: the higher energy band
is conducting while the low energy band is insulating. The
conduction band most likely originates from one of the
double chains furthest from the surface and its carrier
concentration and electronic properties are closer to that
of the bulk, where the chains are known to be metallic
[24,28]. In contrast, the gapped insulating band is most
likely due to the chain layer that is exposed to the surface.
It is almost isolated from the rest of the system and has a
very different carrier concentration. In the rest of this letter,
we present intriguing properties of the conduction band.

In Fig. 1(d), we plot our measured Fermi surface from
the conducting CuO chains. A fascinating feature is the
strong variation of the spectral intensity along the 1D-like
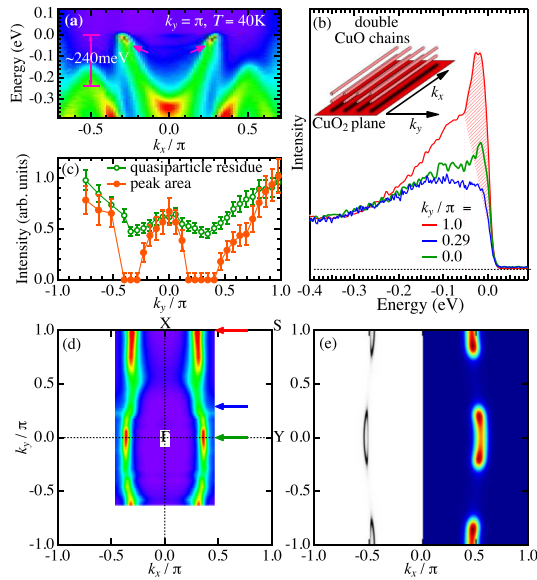Fermi surface. To study this further, we examine in



FIG. 1 (color online). (a) Band dispersion map along the
chains. ($h\nu = 22$ eV) (b) EDCs at three $k_F$'s indicated by arrows
in (d). (c) Quasiparticle residue (spectral intensity integrated
within $\pm 50$ meV of $E_F$) and area of the quasiparticle peak
[illustrated in (b)] along the Fermi surface. (d) Measured
Fermi surface determined by integrating the EDCs within
$\pm 50$ meV of $E_F$ at $T = 20$ K with $h\nu = 33$ eV.
(e) Calculated Fermi surface [2]: zero-energy spectral function
$A(k, 0)$ at $T = 0$ K (left image) and expected ARPES intensity
$I(k, 0)$ (right image).

Fig. 1(b) the typical energy distribution curves (EDCs) at
three $k_F$ points along momentum cuts indicated with
arrows in Fig. 1(d). We find that the quasiparticle peak
is absent in some regions [dark grey (blue) curve in
Fig. 1(b)]. We estimate the spectral weight of the quasi-
particle peak [shaded area in Fig. 1(b)] and plot it in
Fig. 1(c) along with the intensity at $E_F$, which represents
the quasiparticle residue. The absence of a quasiparticle
peak produces six disconnected segments of a quasiparticle
Fermi surface in momentum space [islands of strong in-
tensity in Fig. 1(d)]. This result is in excellent agreement
with a recent ch-DMFT calculation [2], which predicts thin
elongated Fermi pockets in coupled CuO chains. The left
image of Fig. 1(e) shows the result of this calculation. The
authors of Ref. [2] also suggest in the right half of Fig. 1(e)
what these pockets would look like in ARPES, with its
finite energy and momentum resolution. The pockets are so
narrow that the ARPES intensity at the Fermi level is
expected to appear as six arclike segments—as we indeed
see in our data. The location of the calculated islands ($k_x$
value) is different from our data: the calculation assumes
half filling and the experimental situation is close to quarter
filling. Here it is worth mentioning that the calculation
assumes a spinless situation and the model can be viewed
as a caricature of a spin-1/2 model with quarter filling and
a very strong local repulsion [2].

Our results for CuO chains in Y124 are naturally more
complex than those predicted by the ch-DMFT calcula-
tions. In particular we find a significant band renormaliza-
tion effect near the Fermi level that appears as a "kink" in
dispersion [see arrows in Fig. 1(a)] most likely due to a
coupling between the CuO chain electrons and a collective
mode associated with chains. We confirmed that the energy
dispersion with the kink has only a single peak in momen-
tum distribution curves (MDCs) at $E_F$. The energy of the
"dip" in EDC associated with the kink structure has
constant binding energy regardless of the momentum.
These features are all consistent with the bosonic mode
interpretation for the kink and exclude the possibility that
two overlapping bands are the culprit. Furthermore, the
photon energy studies of this feature (not shown) reveal
that the intensities of the low and high binding energy
portion of this feature have the same photon energy de-
pendence. If this feature would originate from two different
bands, their intensities would have different photon energy
dependence due to different matrix element effects.

Now we need to clarify whether or not there is a
relationship between the quasiparticle peaks and the
mode coupling, which may enhance the peak intensity.
Figures 2(a)–2(d) show the band dispersion along the
chains measured at several values of $k_y$ below $T_c$. The
strength of the kink structure in the dispersion changes
dramatically with $k_y$ momentum. The momentum variation
is seen more clearly in Fig. 2(e), where we plot the band
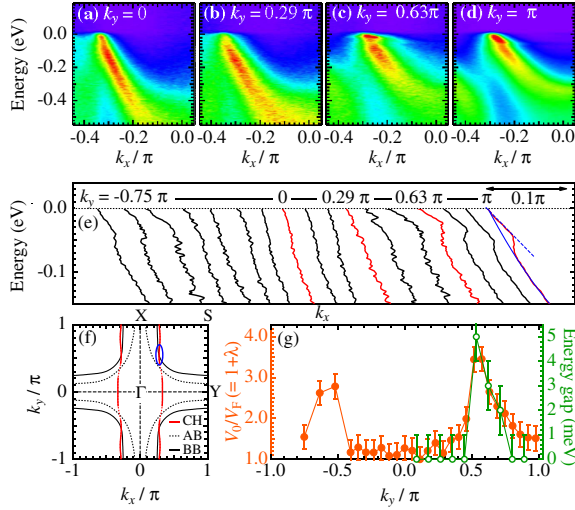dispersion close to $E_F$. We estimated the strength of the

FIG. 2 (color online). (a)–(d) Band dispersion maps along chains. ($T = 20$ K, $h\nu = 33$ eV) (e) Band dispersion plots determined from MDC peak positions. (f) Fermi surface of chains (CH) and plains (AB: antibonding band, BB: bonding band). The superconducting gap region is marked by (blue) circle. (g) Ratio between quasiparticle velocities without and with the mode coupling ($V_0/V_F$) and superconducting gap along Fermi surface. The gap size was estimated from high resolution data at $h\nu = 22$ eV.
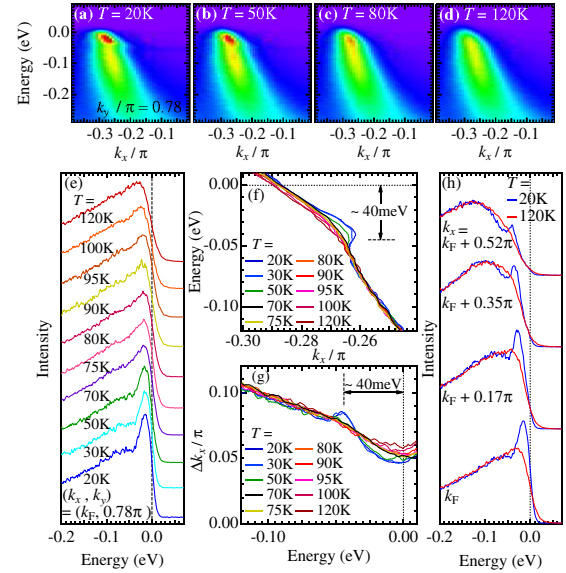


FIG. 3 (color online). (a)–(d) Band dispersion maps at $k_y/\pi = 0.78$ measured at various temperatures from deep below to above $T_c$. ($h\nu = 33$ eV) (e) EDCs at $k_F$, (f) band dispersions determined from MDC peak positions, and (g) MDC widths at various temperatures. (h) EDCs close to $k_F$ below and above $T_c$.

renormalization by taking the ratio of the quasiparticle velocity at the Fermi level without and with the mode coupling $V_0/V_F$, and plot it in Fig. 2(g). $V_F$ is simply the slope of the dispersion data. $V_0$ was estimated as the slope of the parabolic band extrapolated from high energy. Moving from the zone boundary to the center, we find that the ratio ($V_0/V_F$) increases sharply in a narrow momentum range and then drops to almost one [(orange) solid circles, Fig. 2(g)]. This momentum variation is very different from that of the quasiparticle peaks [Fig. 1(c)], indicating that the quasiparticle peaks have no direct relation with the mode coupling. We note that the renormalization effect becomes significant in a region of the Brillouin zone where the chain and plane Fermi surfaces cross each other [see Fig. 2(f)]. In addition, we find the superconducting gap which varies strongly with momentum [(green) open circles, Fig. 2(g)] following the strength of renormalization. The direct relationship between the strength of the renormalization and the value of energy gap is similar to that observed in superconducting $CuO_2$ planes, where these two parameters are maximal at the antinode [18–20]. It seems that electrons in the chains and planes significantly interact with each other via the bosonic mode in a small momentum region [28]. The superconducting gap ($\sim 5$ meV) observed in the chains is significantly smaller than that in planes [29]. This might be because the superconducting gap in the CuO chains is due to a proximity effect originating from the planes [30,31]. It was reported that $c$-axis conductivity remains metallic at low

temperatures in Y124 in the underdoped regime [24,25]. This is in contrast to other underdoped cuprates, which show insulating behavior along the $c$ axis. Furthermore, Y-Ba-Cu-O compounds are characterized by relatively strong three-dimensional superconductivity. Our data strongly suggest that nontrivial electron hopping between the chains and planes plays a significant role in enhancing 3D properties of this most commonly studied high-temperature superconductor.

We investigate the properties of the renormalization effect in more detail. Figures 3(a)–3(d) show the band dispersion at $k_y = 0.78\pi$ measured at various temperatures below and above $T_c$. The EDCs at $k_F$, band dispersion, and MDC widths (related to the scattering rate of the electrons) are plotted as a function of temperature in Figs. 3(e)–3(g), respectively. The renormalization effect is clearly seen at $\sim 40$ meV below $T_c$ and is suppressed above $T_c$, so the effect is tied to the superconductivity. In Fig. 3(h), it is demonstrated that the characteristic peak-dip-hump structure in EDCs close to $k_F$ disappears above $T_c$. The temperature dependence and energy scale of the renormalization effect are similar to those of the bosonic mode observed in superconducting $CuO_2$ planes.

To elucidate the origin of the observed collective mode we measured the band dispersion in 1% Zn-doped Y124 samples, and compared the one for pristine samples. The addition of Zn drastically changes the magnetic environment with no significant effect on the lattice vibrations because of the similar masses of Zn and Cu. ARPES data on pristine and Zn-doped samples measured under exactly the same conditions are shown in Figs. 4(a) and 4(b),
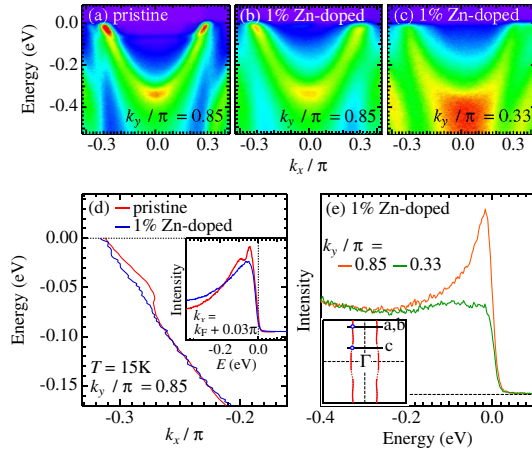
FIG. 4 (color online).   Band dispersion maps for (a) pristine
and (b),(c) 1% Zn-doped sample. The corresponding momentum
cuts are indicated in the inset of (e). (d) Band dispersion plots
determined from MDC peak positions for (a) and (b). Inset
shows EDCs slightly off $k_F$. (e) EDCs at $k_F$'s for (b) and (c).

respectively. The corresponding band dispersion and EDCs
slightly off the $k_F$ are compared in Fig. 4(d). Although the
entire band shape (bottom energy and $k_F$ value) are almost
identical in the both samples, the kink structure and the
peak-dip-hump spectral shape observed in the pristine
samples are effectively absent in Zn-doped samples. This
strongly suggests that the renormalization effect in the
CuO chains has magnetic origin and it is due to coupling
between the electrons and spin fluctuations. A similar Zn-
doping effect is observed in superconducting $CuO_2$ planes
[20] strongly supporting the view that the bosonic mode
has a common origin in CuO chains and $CuO_2$ planes.

Figures 4(b) and 4(c) show the band dispersion mea-
sured along two momentum cuts, where spectra with and
without quasiparticle peaks are observed in pristine
samples, respectively. The corresponding EDCs at $k_F$'s
are plotted in Fig. 4(e). Clearly the kink is absent from
the Zn-doped samples [Fig. 4(d)], but the quasiparticle
peaks remain in the same regions of the Brillouin zone as
the pristine samples. This result supports our idea that the
quasiparticle peaks are not due to a collective mode, but are
due to chain coupling as predicted by the ch-DMFT
calculations.

In conclusion, we observed three intriguing features in
CuO chain band of $YBa_2Cu_4O_8$. One is a quasiparticle
Fermi surface that consists of six disconnected segments.
This is in excellent agreement with the results of ch-DMFT
calculations for coupled 1D chains. Second is a strong
renormalization effect. The properties of this effect are
very similar to those of the bosonic mode observed in the
$CuO_2$ planes. As a third significant result, we observed a
small superconducting gap in CuO chains that is most
likely due to proximity effect originating from the planes.

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