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Observation of Band Renormalization Effects in Hole-Doped High-$T_c$ Superconductors

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We report a systematic high-resolution angle-resolved photoemission spectroscopy on high-$T_c$ superconductors Bi$_2$Sr$_2$Ca$_n$-1Cu$_n$O$_{2n+4}$ ($n = 1–3$) to study the origin of many-body interactions responsible for superconductivity. For $n = 2$ and 3, a sudden change in the energy dispersion, so called “kink”, becomes pronounced on approaching $(\pi, 0)$ in the superconducting state, while a kink appears only around the nodal direction in the normal state. For $n = 1$, the kink shows no significant temperature dependence even across $T_c$. This could suggest that the coupling of electrons with $Q = (\pi, \pi)$ magnetic mode is dominant in the superconducting state for multilayered cuprates, while the interactions at the normal state and that of single-layered cuprates have a different origin.

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It is generally accepted that many-body interactions of electrons plays an essential role in the occurrence of superconductivity. In classical superconductors described well by Bardeen-Cooper-Shrieffer (BCS) theory [1], phonons are regarded to pair two electrons. In cuprate high-$T_c$ superconductors (HTSCs), on the other hand, it has been suggested that other collective excitation mediates the pairing since the superconducting transition temperature ($T_c$) is much higher than those of conventional superconductors. Angle-resolved photoemission spectroscopy (ARPES) with improved resolution has elucidated a key spectral feature indicative of the strong coupling known as kink in the dispersion [2–4]. The behavior of kink has been interpreted in terms of several different excitations, such as longitudinal optical (LO) phonons [3] and a collective magnetic mode [2,4,5]. However, in spite of a general agreement on its importance to the superconductivity, a final consensus on the origin of kink has not been reached. This is due to the lack of systematic ARPES data on the momentum-, temperature-, doping-, and material-dependence of the kink.

In this Letter, we report a high-resolution ARPES study on Bi-family HTSCs (Bi$_2$Sr$_2$Ca$_n$-1Cu$_n$O$_{2n+4}$; $n = 1–3$). The experimental results show that a kink distinctly appears around $(\pi, 0)$ in the superconducting (SC) state and shows a characteristic temperature dependence different from that of the kink near the nodal direction. By analyzing the comprehensive ARPES data, we discuss the origin of two different kinks and their relation to the high-$T_c$ superconductivity.

High-quality Bi$_2$Sr$_2$Ca$_n$-1Cu$_n$O$_{2n+4}$ ($n = 1–3$) single crystals were grown by the traveling solvent floating zone method [6,7]. ARPES measurements were performed using a SCIENTA SES-200 spectrometer with a high-flux discharge lamp and a toroidal grating monochromator at Tohoku University, and with a same-type spectrometer at the undulator 4 m normal incidence monochromator (NIM) beam line at the Synchrotron Radiation Center, Wisconsin. He I$\alpha$ resonance line (21.218 eV) and 22 eV photons were used to excite photoelectrons. The energy and angular (momentum) resolutions were set at 9–15 meV and 0.2 deg ($0.007 \, \text{Å}^{-1}$), respectively. Samples were cleaved in situ in an ultrahigh vacuum better than $5 \times 10^{-11}$ Torr to obtain a clean surface. The Fermi level ($E_F$) of samples was referred to that of a gold film evaporated onto the sample substrate. The samples are labeled by their doping levels (UD for underdoped, OP for optimally doped, OD for overdoped) together with their onset $T_c$. For example, UD100K means an underdoped sample with the $T_c$ of 100 K.

Figure 1 shows ARPES-intensity plots for underdoped Bi$_2$Sr$_2$Ca$_2$Cu$_3$O$_{10}$ with $T_c = 100$ K (Bi2223 UD100K) at the normal and SC states, measured along five cuts in the Brillouin zone (cuts A–E). For cut A at 40 K, the band rapidly approaches $E_F$ from high-binding energy and suddenly bends at 50–80 meV, showing a characteristic kink in the dispersion. The kink is weakened with increasing temperature, but still survives even above $T_c$. In contrast to the relatively small temperature dependence in cut A, a drastic change is observed in the momentum region away from the nodal direction. In cut E just between the nodal direction and $(\pi, 0)$ point [8,9], a sharp kink at 50–80 meV together with opening of the SC gap is clearly seen at 40 K, while the dispersion is almost straight at 140 K. It is noted here that the kink in cut E at the SC state is not due to the opening of the SC gap, because the Bogoliubov quasiparticle band bends smoothly toward higher binding energy near $E_F$ and...
does not make a kink like that in cut E [10]. We find in Fig. 1 that the kink appears only near the nodal direction in the normal state and gradually smears out on approaching $(\pi, 0)$, while the kink becomes more pronounced near $(\pi, 0)$ at the SC state (40 K). This totally opposite behavior of kinks as a function of momentum at two different temperatures above/below $T_c$ suggests that the kink at the nodal direction in the normal state is different from the kink near $(\pi, 0)$ at the SC state.

Figure 2 shows ARPES-intensity plots of Bi2223 (UD100K) as a function of temperature across $T_c$ measured along cuts A and E. For cut E, a strong renormalization of the dispersion is clearly seen at low temperatures below $T_c$, while the temperature-induced change is almost negligible at high temperatures above $T_c$. This strongly suggests that the kink at cut E is closely related to the superconductivity. In contrast, the kink at cut A shows much smaller temperature dependence in the SC state although the kink is slightly enhanced at low temperatures.

In Fig. 3 we show the temperature dependence of the momentum distribution curve (MDC) peak position for $n = 1\text{–}3$ measured along the nodal and the off-nodal direction. For $n = 2$ and 3, the dispersion along the off-nodal cut shows a strong bending behavior below $T_c$, while that above $T_c$ is almost straight with very small temperature dependence. This indicates that the kink around $(\pi, 0)$ disappears around $T_c$ for $n = 2$ and 3, showing a close correlation to the superconductivity. In sharp contrast to the remarkable temperature dependence of kink for $n = 2$ and 3, the dispersion of $n = 1$ shows almost no temperature dependence for both directions. This implies that the electron-mode coupling, which give rise to the strong temperature dependence in $n = 2$ and 3, is absent or very weak in $n = 1$.

In Fig. 4 we plot the maximum value of the real part of self-energy $\text{Re}\Sigma(\omega)^{\text{max}}$, defined as an energy difference between the kink and the linear bare band dispersion which passes the experimental dispersion at $E_F$ and 250 meV (see the inset of Fig. 4) [4]. It is known that $\text{Re}\Sigma(\omega)^{\text{max}}$ serves as a good measure of the coupling strength when $\text{Re}\Sigma(\omega)^{\text{max}}$ comes dominantly from the interaction of electrons with collective excitation [4,12]. As seen in Fig. 4, $\text{Re}\Sigma(\omega)^{\text{max}}$ of $n = 2$ and 3 at the off-nodal direction gradually decreases with increasing temperature for all samples. However, $\text{Re}\Sigma(\omega)^{\text{max}}$ is almost vanished at $T_c$ in optimal- and overdoped samples while it has a finite value even at $T_c$ and still gradually decreases at higher temperatures in underdoped samples. This characteristic behavior of $\text{Re}\Sigma(\omega)^{\text{max}}$ for different dopings resembles the temperature dependence of the magnetic-resonance peak reported by the inelastic neutron scattering (INS) experiment [11]. The peak intensity of the resonance peak of YBa$_2$Cu$_3$O$_{6+\delta}$ with similar $T_c$ [11] is superposed in Figs. 4(b) and 4(c). We find a surprisingly good quantitative agreement between $\text{Re}\Sigma(\omega)^{\text{max}}$ and the resonance-peak intensity. In particular, it is remarked that the resonance peak has a finite intensity even at $T_c$ and gradually decreases with increasing temperature in underdoped samples, in a quite similar manner to the temperature dependence of $\text{Re}\Sigma(\omega)^{\text{max}}$. This indicates that the kink around $(\pi, 0)$ in Bi2212 ($n = 2$) is of magnetic origin [2,4,5]. In contrast to the remarkable temperature dependence of $\text{Re}\Sigma(\omega)^{\text{max}}$ in the off-nodal direction, that of the nodal direction shows much less temperature dependence, as seen in Fig. 4. It is also remarked that $\text{Re}\Sigma(\omega)^{\text{max}}$ in Bi2201 ($n = 1$) shows almost no temperature dependence in both directions in sharp contrast to the multilayered compounds (Bi2212 and Bi2223).
It is thus established that the kink around \((\pi, 0)\) has a close relation to the superconductivity. A possible interpretation of the kink is a coupling of electrons with a magnetic mode for the following reasons. First, it is clear from Figs. 1–3 that the kink at the SC state is stronger near \((\pi, 0)\) than around the nodal direction for \(n = 2\) and \(3\). This indicates that electrons at \((\pi, 0)\) are easily scattered by the mode with a \((\pi, \pi)\) vector [13,14]. This is consistent with the \(Q = (\pi, \pi)\) nature of the magnetic-resonance mode. Second, as shown in Fig. 4, the temperature dependence of the magnetic resonance peak intensity shows an excellent agreement with that of \(\text{Re}\Sigma(\omega)^{\text{max}}\). Third, the absence of a temperature-dependent kink around \((\pi, 0)\) for \(n = 1\) is consistent with the magnetic-mode scenario because a resonance peak has not been observed in Bi2201 [15]. It is expected from the present ARPES results that Bi2223 shows a magnetic-resonance peak similar to that of Bi2212 in the INS experiment, although the INS data are not available at present because of the lack of a large Bi2223 single crystal [16]. The observed dissimilarity in the behavior of kink between single- and multilayered Bi-family compounds implies that the interlayer interaction is essential for the stronger coupling of electrons with magnetic modes as well as for higher \(T_c\). This is supported by INS experiments [17], which show that the resonance-peak intensity of YBCO shows a modulation along \(Q_z\), indicative of a strong coupling between adjacent CuO2 layers [17].

Now we discuss the origin of the kink around the nodal direction at the normal state. We summarize the properties and behaviors of the kink as follows: (1) The kink around the nodal direction survives even above \(T_c\), while the kink around \((\pi, 0)\) disappears around \(T_c\). However, (2) the kink around the nodal direction does not show clear temperature dependence above \(T_c\). (3) A kink in the nodal direction is seen also in materials where a magnetic-resonance peak is absent [3]. There are several candidates responsible for this kink. The first one...
The location in the Brillouin zone and the temperature is the coupling of electrons with LO phonon \[3\].

The last \(Q\) is the broad magnetic excitation observed in the experimental fact that the kink appears strongest in \(n\)–1 states. This suggests that the characteristic temperature dependence below \(T_c\) for Bi2212 and Bi2223 (see Fig. 3). This suggests that the magnetic mode, which is dominant around \((\pi, 0)\), has a finite influence around the nodal direction in the SC state.

In conclusion, we performed a systematic and comprehensive ARPES study on Bi\(_2\)Sr\(_2\)Ca\(_n\)-1CuO\(_{2n+1}\) \((n = 1–3)\) to study the momentum-, temperature-, doping-, and CuO2 layer dependence of the many-body interaction. The experimental results indicate that there are two different kinks in the dispersion. One appears mainly around \((\pi, 0)\) only below \(T_c\) and has a strong temperature dependence. Another appears around the nodal direction both below/above \(T_c\), showing less temperature dependence. The kink around \((\pi, 0)\) is ascribed to the magnetic-resonance mode observed by the INS experiment, while the kink around the nodal direction at the normal state is of a different origin. The characteristic temperature dependence of kinks shows that the coupling of electrons with the magnetic mode is closely related to the superconductivity.

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**FIG. 4** (color). Maximum value of the real part of the self-energy \(\Re \Sigma(\omega)^{\text{max}}\) as a function of temperature measured along the nodal and the off-nodal cut for Bi2201, Bi2212, and Bi2223. The inset shows the definition of the experimentally determined \(\Re \Sigma(\omega)^{\text{max}}\). A vertical solid line on each panel shows the \(T_c\) of sample. The intensity of the resonance peak of YBa2Cu3O6 \(_6\) with similar \(T_c\) [11] is superposed in panels (b) and (c).

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is the marginal Fermi-liquid–like excitation [4]. The temperature-independent behavior of kink at the normal state seems consistent with this interpretation. The second is contribution from the magnetic-resonance mode which survives even above \(T_c\) [11]. However, the experimental fact that the kink appears strongest in the nodal direction is hardly explained in this framework, since the nodal direction is not connected by the \(Q = (\pi, \pi)\) vector of magnetic mode. The third is the broad magnetic excitation observed in the \(Q\)-independent INS [18], which has been proposed to contribute to the kink at the normal state [5]. The last is the coupling of electrons with LO phonon [3]. The location in the Brillouin zone and the temperature-independent nature above \(T_c\) are consistent with the \(Q = (\pi, 0)\) character of the LO phonon [19].

The phonon energy estimated from the INS experiment [19] is 80 meV while the characteristic energy due to the magnetic mode is also 80 meV [40 meV (mode energy) \(+ 40\) meV (SC gap energy)] for optimally doped Bi2212 [14]. This may be the reason for a similar energy scale for two kinks located near nodal direction and around \((\pi, 0)\). It is noted that the kink around the nodal direction shows a finite temperature dependence below \(T_c\) for Bi2212 and Bi2223.

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[8] We do not use the ARPES data around \((\pi, 0)\) for estimating the peak dispersion to avoid possible complication from the flat band, the bilayer splitting [9], and the superlattice bands.
[16] The slightly larger value of \(\Re \Sigma(\omega)^{\text{max}}\) at the off-nodal direction for \(n = 3\) than that for \(n = 2\) suggests that the resonance peak in Bi2223 would be much more intense than Bi2212.