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Universal quasiparticle decoherence in hole- and electron-doped high-$T_c$ cuprates


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We use angle-resolved photoemission to unravel the quasiparticle decoherence process in the high-$T_c$ cuprates. The coherent band is highly renormalized, and the incoherent part manifests itself as a nearly vertical “dive” in the $E$-$k$ intensity plot that approaches the bare band bottom. We find that the coherence-incoherence crossover energies in the hole- and electron-doped cuprates are quite different, but scale to their corresponding bare bandwidth. This rules out antiferromagnetic fluctuations as the main source for decoherence. We also observe the coherent band bottom at the zone center, whose intensity is strongly suppressed by the decoherence process. Consequently, the coherent band dispersion for both hole- and electron-doped cuprates is obtained, and is qualitatively consistent with the framework of Gutzwiller projection.

Understanding the electronic structure and properties in strongly correlated systems, in particular in the high-$T_c$ cuprates, has been a main focus in condensed matter physics over the past two decades. Unlike in simple metals and insulators, the presence of strong correlation makes the predictions of band calculations such as the LDA unreliable. Much of the theoretical understanding, based upon studies of Hubbard-like models, is the existence of strongly renormalized coherent quasiparticle excitations of a much reduced bandwidth $\Delta$ `a la Brinkman-Rice [1] and Gutzwiller wavefunctions [2], and large incoherent background of the Mott-Hubbard [2] type that extends to the bare band edge [2]. Both features have been ubiquitously observed in the cuprates, yet the precise description of the one-particle spectral function over the range of bare bandwidth provided by LDA remained incomplete due to the complexity of this many-body problem. The correlation-induced thermodynamic mass renormalization in the cuprate is $\sim 3$, which can be directly extracted from the renormalized Fermi velocity determined from angle-resolved photoelectron spectroscopy (ARPES) in the prototype Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$. Many ARPES measurements have been performed to determine the band dispersion in the high-$T_c$ cuprates. Remarkably, the band dispersion for the quasiparticle excitations can only be traced up to $\sim 350$ meV, above which the band seems to disappear and the anticipated band bottom at the $\Gamma$ $(0,0)$ point has not been identified [2]. A recent ARPES on the undoped cuprate Ca$_3$Cu$_2$O$_2$Cl$_2$ also found that the renormalized band is truncated around 350 meV, and the incoherent part at high energy seems to follow the bare band dispersion predicted by LDA [2]. It was suggested that the cause of this truncation is the antiferromagnetic fluctuations, with a characteristic energy scale of $2J$, where $J \sim 120 - 160$ meV is the superexchange coupling of the Cu-O square lattice.

In this Letter, we report a systematic APRES study on the complete band dispersion of various cuprates, including hole-doped Pb$_2$Bi$_{2-x}$Sr$_2$CuO$_{6+\delta}$ and electron-doped Pr$_{1-x}$LaCe$_x$CuO$_4$. The most important of our findings is that the truncation energy scale of the coherence-incoherence crossover is not fixed around 350 meV, or $\sim 2J$, instead it is determined by and scales with the bare bandwidth. In the electron-doped cuprates, this crossover along $\Gamma - X$ occurs around $\sim 600$ meV, much larger than the value (350 meV) in the hole-doped ones. At binding energies above the crossover, the incoherent part of the spectrum takes the form of a nearly vertical dispersion around a fixed crystal momentum $k$, and approaches the bare band bottom predicted by LDA. In addition, we observe for the first time the bottom of the renormalized band whose intensity is strongly suppressed. The complete determination of the coherent part of the occupied Cu$d_{3z^2-r^2}$ band enables us to provide the tight-binding parameters and compare to the more realistic quasiparticle dispersion calculated from models with strong local correlation. We find that the renormalized dispersion obtained from the Gutzwiller projected wavefunction approach to the $t - J$ like models is a promising candidate for the observed low energy quasiparticle band.

High quality single crystals of cuprates Pb$_2$Bi$_{2-x}$Sr$_2$CuO$_{6+\delta}$ (Pb-Bi2201), Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ (Bi2212), and Pr$_{1-x}$LaCe$_x$CuO$_4$ (PLCCO) were prepared by the traveling solvent floating zone method, and some were annealed subsequently. ARPES experiments were performed at the Synchrotron Radiation Center, WI, and the Advanced Light Source, CA. High-resolution undulator beamlines and Scienta analyzers with a capability of multi-angle detection have been used. The energies of photons were carefully chosen in order to enhance certain spectral features. The energy resolution is $\sim 10 - 30$ meV, and the momentum resolution $\sim 0.02$ Å$^{-1}$. All the samples were cleaved and
measured in situ in a vacuum better than $8 \times 10^{-11}$ Torr at low temperatures (14 - 40 K) on a flat (001) surface, and all the spectra shown below have been reproduced on multiple samples.

We start with a set of spectra along $\Gamma-X$ on a hole-doped Pb$_2$Bi$_{2-x}$Sr$_2$CuO$_{6+y}$ (overdoped $T_c \sim 7$K), as shown in Fig. 1. The reason we choose this material is that the Pb substitutions remove the superlattice modulation in Bi-O plane, which often complicates ARPES spectra. The spectra were taken along $\Gamma-X$ in the second Brillouin zone (BZ) using 57-eV s-polarized ($\hat{A} \parallel \Gamma X$) photons to enhance various features at high binding energy (> 350 meV). In Fig. 1a, one can easily follow the dispersive band at low energy (< 350 meV). This band is the well-know Zhang-Rice singlet, with the predominant Cu$_3$드$a_{2-g}$-O$_2$prü,y antibonding orbital. While the Fermi vector $k_F$ is almost the same as the one predicted by LDA, as shown in Fig. 1d, its dispersion velocity $v_F$ ($\sim 2.1$ eVÅ) is much smaller than the LDA value ($\sim 5.2$ eVÅ), consistent with previous ARPES results. Note that the Fermi velocity $v_F$ ($\sim 1.6$ eVÅ) at $k_F$ is even smaller due to a further renormalization by the observed nodal kink at $\sim 70$ meV, which is difficult to visualize at the large energy scale in Fig. 1.

At higher binding energy (> 350 meV), the spectrum becomes ill-defined. While the intensity plot (Fig. 1a) seems to indicate that the spectra abruptly “dive” almost vertically from 350 meV to at least 1 eV, this diving behavior does not expressed itself as a peak in the energy distribution curves (EDCs) (Fig. 1b). Instead, an enhancement in the EDC background is observed at the $k$-location of the dive around $(\pi/4, \pi/4)$ and equivalent $k$ points in other BZs, as shown in Fig. 1f where the EDC at the dive location (# 2, as marked in Fig. 1a) has a higher background than its neighboring EDCs (e.g., # 1 and # 3). The diving behavior is reflected more clearly in the momentum distribution curves (MDCs), as shown in Figs. 1d where the MDCs seem to maintain their peak shape. Since the dive completely loses the peak (or pole) structure in energy, strictly it is no longer a band. Nevertheless, it is likely the incoherent part of the Cu$_3$드$a_{2-g}$-O$_2$prus,y (or ZRS) spectrum, since it maintains the $d_{x^2-y^2}$ symmetry. We have verified this symmetry, as shown in the inset of Fig. 1f, where both the coherent band and the dive are suppressed by $p$-polarized light ($\hat{A} \perp \Gamma X$). This is due to a well-known ARPES selection rule. In addition, we have also observed that the intensity ratio between these two features is roughly a constant when we change $s$ and $p$ polarization components, supporting that the dive is the incoherent part of the band.

So far we have shown that the coherent ZRS band disperses to a certain energy (~ 350 meV) and then abruptly switches to the incoherent part at the higher energies. However, if we take a closer look at the EDCs in the vicinity of $\Gamma$, we observe the smooth continuation of the coherent band, which reaches the bottom around 0.5 eV at $\Gamma$, as shown in Fig. 1c. This is the long-sought-after renormalized band bottom, and the reason we can observe it for the first time is due to several combined factors such as the superlattice free sample, a proper photon energy, and the second BZ, all of which enhance the intensity of the high-energy features. We note that the coherent band starts to lose its intensity at the same energy where the incoherent diving pattern begins to form, indicating a weight transfer between the coherent and incoherent parts. The bottom of the coherent band can be also visualized, as shown in Fig. 1d, from the second derivative of the intensity with respect to energy which enhances broad horizontal features. In Fig. 1d, we compare the dispersion of the coherent band with the calculated one from LDA, along with the dispersion extracted from MDCs. It is clear that the coherent band, with a well-defined parabolic shape, is highly renormalized, and the vertical feature is likely the incoherent part, which approaches the bottom of the bare band.

We have observed very similar behaviors of the coherence-incoherence crossover in the bilayer system Bi$_2$Sr$_2$CaCu$_2$O$_{8+x}$, except the superlattice in this material makes it difficult to observe the bottom formation of the coherent band at $\Gamma$. Like in Pb-Bi2201, the incoherent part in Bi2212 deviates from the coherent part around 350 meV, and approaches almost vertically the bare band bottom around 1.5 eV. Since the 350 meV energy scale of the coherence-incoherence crossover has been attributed to the antiferromagnetic fluctuations whose characteristic energy scale $2J$ has a similar value, it is natural to...
check if a similar coherence-incoherence crossover exists in the electron-doped cuprates. We have searched for this crossover on various electron-doped cuprates, and the main results are presented in the following two figures.

We first show, in Fig. 2, the dispersion of the electron-doped cuprate Pr$_{0.88}$LaCe$_{0.12}$CuO$_4$ ($T_c \sim 23$ K) near $\Gamma - X$ using 22-eV $p$-polarized photons. Since the band intensity exactly along $\Gamma - X$ is highly suppressed due to the selection rule mentioned above, we choose to display the dispersion along the parallel direction slightly away from the $\Gamma - X$ direction, as indicated in the inset of Fig. 2b. A quick examination of the plots of Fig. 2 reveals a major difference to the hole-doped materials: the coherent band in PLCCO extends to a much higher binding energy. The separation of the incoherent part occurs around 0.6-0.7 eV, which also forms a diving pattern at higher binding energy, as seen in both the intensity plot in Fig. 2a and the MDCs plot in Fig. 2c. We note that the diving pattern appears to be shorter than the one in the hole-doped cuprates. We believe that this is due to the hybridization between the Cu$3d_{x^2-y^2}$ band and some other bands, as predicted by LDA calculations and shown in Fig. 2b (dashed green curves). The bare Cu$3d_{x^2-y^2}$ band, while not mixing with those bands, reaches the bottom around 2.1 eV, as indicated in Fig. 2b (solid black curves) $^{[15]}$. In comparison, the coherent part has its band bottom around 0.8 eV, indicating a mass renormalization of 2.5, similar as in the hole-doped case.

The different energy scale of the coherence-incoherence crossover in the electron-doped cuprates, as observed in PLCCO and confirmed in other electron-doped materials, such as Pr$_{2-x}$Ce$_x$CuO$_4$ and Nd$_{2-x}$Ce$_x$CuO$_4$, argues strongly against the antiferromagnetic scenario. Instead, the same mass renormalization ratio in both cases suggests that this energy scale may be related to the bare bandwidth. This is also true in the electron-doped material along another high-symmetry direction, $M - X$, as can be seen in Fig. 3. It is well known that the van-Hove saddle point shifts to a much higher binding energy ($\sim 0.4$ eV) in the electron-doped cuprates $^{[17,18]}$. Over the wide energy range, the Cu$3d_{x^2-y^2}$ band dispersion along $M - X$ in PLCCO has many similarities to the band along $\Gamma - X$ in Bi2201, as shown in Fig. 3. The coherent part along $M - X$ in PLCCO, while being quite broad due to the possible stronger interactions near the antinode, extends to an energy scale ($\sim 0.25$ eV) when the incoherent part takes a dive. The bottom of the coherent part at $M$ is estimated to be $\sim 0.3$ eV, and the bare band position at $M$ is calculated by LDA to be $\sim 0.7$ eV. For comparison, we draw both intensity plot and second derivative plot of Pb-Bi2201 in the left panels of Fig. 3 in a slightly reduced energy scale. We also notice that there is a small kink at $\sim 70$ meV along $M - X$ in PLCCO, which resembles the well-know and much-debated nodal kink in the hole-doped cuprates $^{[12,13]}$. We caution that the origin of the antinodal kink in PLCCO may not be the same as the antinodal one in the hole-doped case, and call for more systematic studies.

We have measured band dispersion along many directions in the BZ for various hole- and electron-doped cuprates. In Fig. 4, we summarize our main results as a comparison between the coherent band dispersion and the bare band dispersion predicted by LDA along several high-symmetry directions, for both Pb-Bi2201 ($T_c \sim 7$...
likely the result of strong local correlations that frustrate the kinetic energy. This is overall consistent with the Gutzwiller projected wavefunction approach to simple models of doped Mott insulators. Detailed comparisons would require measurement of the doping dependence of the renormalized bandwidth, which is more difficult to determine due to the doping dependent shift of the chemical potential. More systematic studies are needed to clarify this issue. Most surprisingly, we find that the energy scale associated with the coherence-incoherence crossover is determined by a fraction of the bare band bottom energy and is in general different from the antiferromagnetic exchange energy $2J$, ruling out the latter as the main cause of quasiparticle decoherence at high binding energies. Moreover, it appears more universal that the incoherent spectrum beyond the decoherence energy takes a vertical dive with a nearly fixed $k \sim (\pi/4, \pi/4)$, approaching the bottom of the bare band in what seems to be the “cheapest” way for the renormalized quasiparticles to return to their bare form. The origin of these unexpected behaviors is largely unknown and demands more understanding of the interplay between the coherent quasiparticle and collective excitations and the dominant incoherent processes in the spectral function, which has been one of the central challenges in the physics of strong correlations.

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*Note added:* During the preparation of this manuscript, we became aware of three preprints reporting independently ARPES results of band dispersion over a large energy scale on the hole-doped cuprates [20, 21, 22].