Normal state electronic structure in the heavily overdoped regime of Bi$_{1.74}$Pb$_{0.38}$Sr$_{1.88}$CuO$_{6+d}$ single-layer cuprate superconductors

K. Yang$^1$, B. P. Xie$^3$, D. W. Shen$^1$, J. F. Zhao$^1$, H. W. Ou$^1$, J. Wei$^1$, S. Wang$^1$, Y. H. Wang$^1$, D.H. Lu$^2$, R. H. He$^2$, M. Arita$^3$, S. Qiao$^3$, A. Ino$^3$, H. Namatame$^3$, M. Taniguchi$^{1,4}$, F. Q. Xu$^5$, N. Kaneko$^6$, H. Eisaki$^6$, D.L. Feng$^6$

$^1$Department of Physics, Applied Surface Physics State Key Laboratory, and Synchrotron Radiation Research Center, Fudan University, Shanghai 200433, China
$^2$Stanford Synchrotron Radiation Laboratory, Stanford University, Stanford, CA 94305, USA
$^3$Hiroshima Synchrotron Radiation Center, Hiroshima University, Hiroshima 739-8526, Japan
$^4$Graduate School of Science, Hiroshima University, Hiroshima, Hiroshima 739-8526, Japan
$^5$National Synchrotron Radiation Laboratory, University of Science & Technology of China, Hefei 230027, Anhui, China and AIST, 1-1-1 Central 2, Umezono, Tsukuba, Ibaraki, 305-8568 Japan.

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We explore the electronic structure in the heavily overdoped regime of the single layer cuprate superconductor Bi$_{1.74}$Pb$_{0.38}$Sr$_{1.88}$CuO$_{6+d}$. We found that the nodal quasiparticle behavior is dominated mostly by phonons, while the antinodal quasiparticle lineshape is dominated by spin fluctuations. Moreover, while long range spin fluctuations diminish at very high doping, the local magnetic fluctuations still dominate the quasiparticle dispersion, and the system exhibits a strange metal behavior in the entire overdoped regime.

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The high-$T_c$ cuprate superconductors (HTSC’s) have been studied for almost 20 years$^{1}$ Anomalous and complicated phenomenology in the underdoped regime of HTSC’s such as pseudogap$^2$, resonant modes in spin fluctuation spectra$^3$ and possible charge ordering$^4$ have led to a broad spectrum of theoretical proposals from the very conventional BCS-type models$^5$ to the very exotic ones involving various gauge fields$^6$. Recent angle resolved photoemission spectroscopy (ARPES) experiments resolved kinks of the quasiparticle dispersions in both nodal and antinodal region of the Brillouin zone$^{7,8,9,10,11,12,13}$. Whether these kinks are originated from electron-phonon or electron-magnon interaction is currently debated$^{9,10,11,12,13,14}$. Nevertheless, the role of phonon in high temperature superconductivity is being revisited$^{15}$.

To date, most experimental studies have been focusing on the anomalous, and certainly interesting, underdoped regime. On the other hand, although to be validated by experiments, the overdoped half of the phase diagram, particularly the heavily overdoped regime, is considered to be a “normal” metal regime where correlations are negligible. The electronic structure in this regime was seldom studied$^{16,17,18,19}$. To build a comprehensive picture of high temperature superconductivity, it is crucial to study the properties of the entire overdoped regime, particularly the heavily overdoped regime, where little data is available at this stage. By examining the overall picture, one hopefully can understand the complications in the HTSC phenomenology better and resolve some of the current controversies, and thus sort out properties that are essential for the high temperature superconductivity.

In this paper, we report a systematic ARPES study of the electronic structure in the heavily overdoped regime of HTSC’s up to the extreme doping level where the superconductivity vanishes (referred as ultra-overdoped regime hereafter). Our data indicate that lattice effect dominates the nodal quasiparticle scattering, while the spin fluctuations dominate the antinodal region. Although long range spin fluctuations diminish at high doping, the local magnetic fluctuations still dominate the quasiparticle dispersion, and correlations are still strong.

High quality superstructure-free Bi$_{1.74}$Pb$_{0.38}$Sr$_{1.88}$CuO$_{6+d}$ (Pb-Bi2201) single crystal was grown by floating-zone technique. Unlike Bi$_2$Sr$_2$CaCu$_2$O$_{8+d}$ (Bi2212), Pb-Bi2201 is a single-layer cuprate and can be doped into much higher doping level. Through Oxygen or Argon annealing, we have prepared overdoped samples with superconducting phase transition temperature $T_c$’s (dopings) of 0K (0.27), 5K (0.26), 7K (0.258), 10K (0.252), 16K (0.24) and 22K (0.25), where the hole concentration $x$’s are estimated based on the empirical formula $T_c = T_{c,opt}[1-82.6(x-0.16)^2]^{20}$ and $T_{c,opt} = 34K$ for Bi2201. For comparison, we also studied a Pb-free optimally doped Bi2201 ($T_c = 34K$, $x = 0.16$). Transition widths of these samples are typically $1 \sim 2K$. Moreover, unlike La$_{2-x}$Sr$_x$CuO$_4$ (LSCO), the cleavage surface of Bi2201 is non-polar and stable, suitable for angle resolved photoemission studies. ARPES experiments were performed at the Beamline 5-4 of Stanford Synchrotron Radiation Laboratory (SSRL), and Beamline 9 of Hiroshima Synchrotron Radiation Center (HSOR). Both beamlines are equipped with a Scienta SES200 electron analyzer, with a typical angular resolution of 0.3° and an energy resolution of 10 meV. If not specified, the data were taken at $10 \sim 15K$ above $T_c$ with 22.7eV photons.

We start with the examination of the nodal quasiparticle behavior. Fig. 1 shows the nodal photoemission intensity map, where a kink in dispersion is clearly visible.
FIG. 1: (a) Normal state photoemission intensity as a function of energy and nodal momentum for $x = 0.26$. The inset on the left is MDC’s at different binding energies that can be fit well with a Lorentzian. The dispersion is extracted through the MDC analysis and shown as the thick dashed line. The inset on the right is the band velocity based on the dispersion, where it is a fixed value at low or high binding energies defined as $V_{\text{low}}$ or $V_{\text{high}}$. (b) Dispersion extracted from MDC analysis in the nodal direction for various doping levels. Inset: Dispersions for $x = 0.225$ and $T=30, 100, 200$K; $x = 0.24$ and $T=60, 120, 190, 250$K; and $x = 0.27$ and $T=10, 100, 150, 200, 250$K. $V_{\text{low}}$, $V_{\text{high}}$ and $Z \equiv V_{\text{low}}/V_{\text{high}}$ as a function of doping.

even for the $x = 0.26$ high doping level.27 As illustrated by the thick dashed line, one can extract the effective band velocities $V_{\text{high}}$ and $V_{\text{low}}$ for dispersion below and above the kink energy scale respectively (inset of Fig. 1b). Dispersions and effective band velocities for various dopings are displayed in Figs. 1b and 1c respectively. Similar to the LSCO system, $V_{\text{low}}$ here is also almost doping independent, while $V_{\text{high}}$ decreases slowly with increased doping. Recently, it has been shown that the coherent quasiparticle spectral weight $Z$ can be estimated as $V_{\text{low}}/V_{\text{high}}$ for cuprates28 which increases from 0.4 at $x = 0.225$, to 0.53 at $x = 0.27$(see Fig. 1b). These agree quite well with the calculations by Paramekanti et al.22 At different temperatures (inset in Fig. 1b), the dispersion varies very little, indicating that $Z$ does not decrease with rising temperature. Therefore, in the highly overdoped regime of Bi2201, we do not observe a coherent-incoherent transition with increasing temperature as a recent study of overdoped Bi2212 claimed.22

Fig. 2a compares the photoemission spectrum at nodal Fermi crossing and that at $(\pi, 0)$ for four different dopings ranging from the optimal doping level to ultra-overdoped $T_c \approx 0$K sample. Remarkably, the $(\pi, 0)$ spectrum sharpens up dramatically with increased doping,

while the nodal spectral linewidth is quite doping inde-
pendent. At very high doping, the \((\pi, 0)\) spectrum appears to be even sharper than the nodal spectrum. The full-width-half-maximum (FWHM) of these spectra are plotted in Fig.2b, as solid symbols. After removing the energy broadening from finite energy resolution and angular resolution, which is significant in nodal direction due to the fast dispersion \(^{28}\) one obtains the intrinsic energy width shown as open symbols. The scattering rate at \((\pi, 0)\) almost decreases by a factor of five in a linear fashion, while the scattering of the nodal quasiparticles remains roughly constant. In the ultra-overdoped regime, the nodal and \((\pi, 0)\) quasiparticles have the same linewidth, \textit{i.e.}, the scattering across the Fermi surface becomes isotropic.

Based on the above experimental observations, one can retrieve information on the interactions between electrons and bosons in the nodal and antinodal regions. In cuprates, the possible candidates for the bosons are phonons and spin excitations. For the nodal quasiparticles, the linewidth is almost doping independent, while \(Z\) increases with doping. This peculiar behavior resembles the photoemission spectrum of Hydrogen molecules, where the vibration modes take the quasiparticle spectral weight from the main peak and redistribute it in multiple mode energies away without affecting the main peak linewidth \(^{27}\). In solid, as simulated in Fig.2d and 2e, it is only when electrons interact with \textit{discrete} bosonic modes with frequencies larger than the original quasiparticle width, could the quasiparticle keep a fixed width while its spectral weight increases with weakening coupling strength. Half-breathing phonon maybe is a candidate to explain our data, it was suggested to interact strongly with the nodal quasiparticles in Bi2212 system \(^9,14\). Moreover, since phonon spectrum does not vary significantly with doping, the increasing screening of electron-phonon interactions can explain the moderate 30% increase of \(Z\) from \(x = 0.225\) to 0.27. On the other hand, we found that in Fig.2f-i, because the spin excitation is a broad spectrum starting from zero frequency in the normal state \(^{28,29}\), its scattering with electrons causes the resulting spectral linewidth a large doping dependence. Furthermore, spin excitation spectral weight drops rapidly to a negligible level at high doping \(^{28}\), which is hard to count for the loss of 47% (\textit{i.e.} 1 \(- Z\)) of the nodal coherent quasiparticle weight for \(x = 0.27\). Therefore, these observations indicate that optical phonons may dominate the scattering of quasiparticles in the nodal region.

Contrary to the nodal case, the \textit{continuously} fast decreasing \((\pi, 0)\) linewidth with doping (Fig.2b) can be explained by the simulation in Fig.2f-i. The broad \((\pi, 0)\) spectrum at optimal doping can be attributed to the strong scattering from the antiferromagnetic fluctuations near \((\pi, \pi)\) (Fig.2g) \(^{28}\). Consistently, when spin fluctuations are significantly weaker in the ultra-overdoped regime as shown by recent neutron scattering data (Fig.2h) \(^{28}\), spectral linewidth gradually recovers its original quasiparticles width (Fig.2i), eventually resulting in an isotropic linewidth across the Fermi surface for \(T_c \sim 0K\). Therefore, the doping and momentum dependence of the quasiparticle lifetime indicate the dominant role of spin fluctuations to the antinodal quasiparticles. As for phonon effects in this region, the out-of-plane \(B_{1g}\) buckling phonon was suggested to interact strongly with the antinodal quasiparticles in bilayer systems due to the nonzero crystal field along \(c\)-axis at the \(CuO_2\) planes \(^{13,14}\). However, for single layer Bi2201, the surroundings of the \(CuO_2\) plane are symmetric, thus the crystal field induced electron-buckling phonon coupling is negligible in Bi2201. For the in-plane half-breathing phonon, it has been suggested that it only interacts weakly with the electrons in the antinodal region \(^{15}\). However, we note that at ultra-overdoping, when spin fluctuations diminish, effects of other phonons might become relatively pronounced in the quasiparticle lineshape (not included in Fig.2i for simplicity).

Having studied the nodal and \((\pi, 0)\) quasiparticles, we now turn to the overall dispersion. Fig.3 (a-c) present the normal state ARPES spectra measured on the ultra-overdoped \(x = 0.26\) sample along the high symmetry directions of the first Brillouin zone. Tracking the peak position of the spectrum, the quasiparticle dispersion is plotted in false color in Fig.3 (d) for \(x = 0.26\) and (e) for \(x = 0.16\) for comparison, which shows that the
The highly overdoped system possesses both strong correlation and well defined quasiparticle. The energy dependence of the nodal quasiparticle scattering rate, $\Delta E \equiv V \times \Delta k$, is plotted in Fig. 4b for two dopings, where $V$ is the band velocity indicated in the inset of Fig. 1. The shaded regions correspond to the kink, which gives an upturn in scattering rate due to electron-phonon interactions, where these bosons are most likely phonons as discussed above. The low energy region can be fit with a power law function, $\Delta E \sim \omega^\alpha$, but $\alpha$ varies from 1 to 3, depending on the choice of the fitting energy window. Meanwhile, the high energy portion above the kink region is always linear. As a function of temperature, the in-plane resistance is plotted in Fig. 4d together with the nodal quasiparticle scattering rate at Fermi energy. Close-to-linear behavior is observed for $x = 0.225$, while for $x = 0.27$, a superlinear temperature dependence is observed, $\rho \sim T^{1.35}$. Similarly, early resistivity studies of ultra-overdoped $\text{Tl}_2\text{Ba}_2\text{CuO}_6+\delta$ have shown superlinear behavior as well\cite{2}. These temperature dependence behavior and the interesting energy dependence indicate that the system is still “strange metal” state in the ultra-overdoped regime.

The non-Fermi liquid behavior near the optimal doping was related to a possible quantum critical point in the vicinity\cite{35,36,37}. The transition from a marginal Fermi liquid behavior toward a more Fermi-liquid-like behavior with tuning of the doping does resemble the quantum critical phenomena observed in $\text{Sr}_3\text{Ru}_2\text{O}_7$ and $\text{YbRh}_2\text{Si}_2$\cite{38,39}. Moreover, in various doping levels and temperatures that were sampled, we so far do not observe any abrupt change in the electronic structure that might be related to a first order transition. Whether or not there is one or more quantum critical points still needs more decisive evidence.

The nodal quasiparticles display many doping-insensitive properties such as the linewidth, $\nu_{low}$. We find them not affected by the long range magnetic fluctuations. Since nodal quasiparticles are responsible for many transport properties, our observations put strong constraints to theories of transport. For the antinodal region where the gap is the largest, the data suggest that long range magnetic fluctuations play an important role. The fact that $d$-wave superconductivity vanishes when the quasiparticle inverse lifetime across the Fermi surface becomes isotropic is very intriguing. Moreover, the quasiparticle dispersion is renormalize by roughly a factor of $x$ from the bare band, indicative of that the local magnetic correlations are still surprisingly strong up to the ultra-overdoped regime\cite{40}.

We conclude by pointing out that the ultra-overdoped regime exhibits many unconventional behaviors that may be fundamentally related to the mechanism of high temperature superconductivity, which calls for more comprehensive theory that could explain the phenomenology over the entire doping range.

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Electronic address: dlfeng@fudan.edu.cn

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