

Effect of spin excitations on the property of quasiparticles in electron-doped cuprate superconductors

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It is proposed that the 50–70 meV dispersion anomaly (kink) in electron-doped cuprates revealed by recent angle-resolved photoemission spectroscopy experiments is caused by coupling with the spin fluctuation. We elaborate that the kink exists both along nodal and antinodal directions, and both in the superconducting and normal state. The renormalized effect for the density of states is also studied and the hump feature outside the superconducting coherent peak is established, consistent with recent scanning tunneling microscopy experiments.

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Although high-temperature superconductivity in cuprates was discovered more than twenty years ago, the mechanism of their unusually high critical temperatures has not yet been clarified.¹ An insightful view may be obtained through the understanding of the role played by certain collective excitations by studying the renormalized single-particle properties. Experimentally, the angle-resolved photoemission spectroscopy (ARPES) and scanning tunneling microscopy (STM) have been powerful tools for providing the electronic structure and probing the interaction of the quasiparticle with certain boson modes.

The superconductivity in cuprates can be achieved by doping either holes or electrons into parent antiferromagnetic (AF) Mott insulators. One of the most important features in hole-doped cuprates revealed by the ARPES experiments is the slope change in the quasiparticle dispersion (kink) from the momentum distribution curve (MDC).² The kink is observed along both nodal and antinodal directions at the energies about 40–80 meV. In the past few years, the origin of the kinks attracted intensive study both theoretically and experimentally because it speculated some kind of interaction which might act as the mysterious glue for Cooper pairs. Two possible bosonic modes, namely, phonon³ and spin-resonance modes revealed by neutron-scattering experiments,⁴ have been proposed to account for the dispersion kink. Theoretically it seems that both electron-phonon interaction⁵ and the coupling of the spin-resonance mode^{6–8} can reproduce the dispersion kink. Unfortunately, these two modes could have similar energies; thus it is difficult to distinguish between the two. Up to now no consensus has yet been reached. On the other hand, STM experiments also identified the existence of the bosonic mode in the hole-doped cuprates but the origin is also under debate.^{9–11}

In the past few years, more and more attention has been turned to the electron-doped cuprates. It is well known that the electron-doped materials exhibit different behaviors from that of hole-doped ones, namely, they usually have lower superconducting (SC) transition temperature and narrower SC doping range. Therefore, the spin-resonance energy is much less, namely, only about 10 meV (Refs. 12 and 13) revealed by the neutron-scattering experiments. On the other hand, the phonon energies are expected to be similar to those of hole-doped ones. Thus the energies of these two modes

are quite different so that their contributions should be easily separated by experiments. Moreover, earlier ARPES experiments in the electron-doped cuprates did not observe the kink along the nodal direction; only the antinodal kink with the energy about 50–70 meV was observed.^{14–16} Very recently, it was reported by several groups that the kinks exist in several families of electron-doped cuprates, both along the nodal^{17–20} and antinodal directions,^{17,18} with the energy being 50–70 meV. Moreover the kinks depend weakly on the doping level and exist even in the normal state. Another renormalized effect revealed by the experiments is the peak-dip-hump structure in the energy distribution curve (EDC),¹⁸ namely, the EDC line shapes display a sharp quasiparticle peak near the Fermi energy E_F along the antinodal direction. This peak terminates and is accompanied with a dip at the energy about 50 meV. The peak width decreases when approaching the Fermi energy. A faint humplike feature is also revealed in the nodal direction. Because the kink energy is much greater than the resonance energy, the spin-resonance peak in fact does not exist in the normal state. Thus it was proposed that the phonon should account for the dispersion kink.^{17–20} On the other hand, a distinct bosonic mode of the energy about 10 meV has also been reported by the STM experiment in electron-doped cuprates.²¹ It is proposed that the mode is caused by spin fluctuations rather than phonons.

In this paper, the spectral function and density of states in electron-doped cuprates observed by experiments^{17–21} can be reproduced by only considering the coupling between the spin excitations and the quasiparticle. We assume phenomenologically that the spin excitations are from spin fluctuations and the retarded Green's function $G(\mathbf{k}, \omega)$ is a function of the bare normal-state quasiparticle dispersion $\varepsilon_{\mathbf{k}}$, the SC order-parameter $\Delta_{\mathbf{k}}$, and the self-energies $\Sigma(\mathbf{k}, \omega)$ due to the coupling of spin fluctuations.^{22–24} The bare normal-state quasiparticle dispersion is expressed by

$$\begin{aligned} \varepsilon_{\mathbf{k}} = & -2t_1(\cos k_x + \cos k_y) - 4t_2 \cos k_x \cos k_y \\ & - 2t_3(\cos 2k_x + \cos 2k_y) \\ & - 4t_4(\cos k_x \cos 2k_y + \cos k_y \cos 2k_x) \\ & - 4t_5 \cos 2k_x \cos 2k_y - t_0, \end{aligned} \quad (1)$$

with $t_{0-5} = -82, 120, -60, 34, 7,$ and 20 meV. This single-

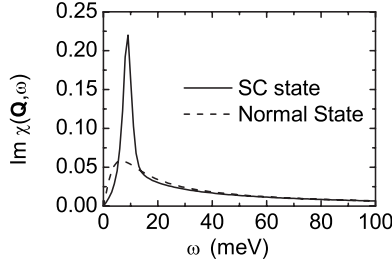


FIG. 1. The imaginary part of the spin susceptibility versus the energy ω at the AF momentum $Q=(\pi, \pi)$ in the SC state and normal state, respectively.

particle dispersion was used by Ref. 25 to fit the ARPES experiments in electron-doped cuprates.¹⁵

The SC order parameter is chosen to have d -wave symmetry, namely,

$$\Delta_{\mathbf{k}} = \Delta_0(\cos k_x - \cos k_y)/2. \quad (2)$$

The spectral function of the electrons can be calculated from the retarded Green's function as $A(\mathbf{k}, \omega) = -(1/\pi)\text{Im} G_{11}(\mathbf{k}, \omega + i\delta)$. Here the Green's function G_{ij} ($i, j=1, 2$) is calculated by Dyson's equation in the Nambu representation (2×2 matrix), namely,

$$\hat{G}(\mathbf{k}, \omega + i\delta)^{-1} = \hat{G}_0(\mathbf{k}, \omega + i\delta)^{-1} - \hat{\Sigma}(\mathbf{k}, \omega + i\delta). \quad (3)$$

The bare Green function of the electron \hat{G}_0 is expressed by

$$\hat{G}_0^{-1}(\mathbf{k}, \omega) = \begin{pmatrix} i\omega - \varepsilon_{\mathbf{k}} & -\Delta_{\mathbf{k}} \\ -\Delta_{\mathbf{k}} & i\omega + \varepsilon_{\mathbf{k}} \end{pmatrix}. \quad (4)$$

The self-energy due to spin fluctuation is written as²⁶

$$\hat{\Sigma}(\mathbf{k}, i\omega) = \frac{1}{\beta N} \sum_q \sum_{i\omega_m} g^2 \chi(\mathbf{q}, i\omega_m) \hat{\sigma}_3 \hat{G}_0(\mathbf{k} - \mathbf{q}, i\omega - i\omega_m) \hat{\sigma}_3, \quad (5)$$

where $\hat{\sigma}_3$ is the Pauli matrix. $\chi(\mathbf{q}, i\omega_m)$ is the spin susceptibility in the random-phase approximation (RPA), namely,

$$\chi(\mathbf{q}, \omega) = \frac{\chi_0(\mathbf{q}, \omega)}{1 + U_{\mathbf{q}} \chi_0(\mathbf{q}, \omega)}. \quad (6)$$

Here $U_{\mathbf{q}} = U_0(\cos q_x + \cos q_y)$ consistent with the t - J type model. $\chi_0(\mathbf{q}, \omega)$ can be calculated from the fermionic bubble,

$$\chi_0(\mathbf{q}, \omega) = -\frac{1}{\beta N} \sum_{\mathbf{k}, i\omega_m} \text{Tr}[\hat{G}_0(\mathbf{k}, i\omega_m) \hat{G}_0(\mathbf{k} + \mathbf{q}, i\omega + i\omega_m)]. \quad (7)$$

In the following presented results, we set $U_0 = 260$ meV and $g = 360$ meV.²⁷⁻²⁹ The temperatures and gaps in the SC and normal states are $T = 0.5$ meV and $\Delta_0 = 10$ meV, and $T = T_c = 2.3$ meV and $\Delta_0 = 0$, respectively. We have checked numerically that the main results are not sensitive to the choice of the parameters.

The imaginary parts of the spin susceptibilities as a function of the energy ω are plotted in Fig. 1. A sharp resonance peak is seen in the SC state at the energy about Ω_r ,

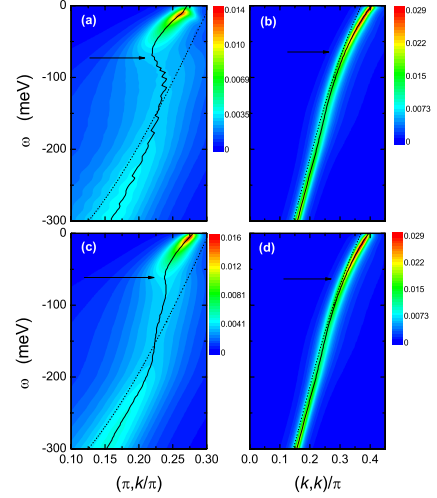


FIG. 2. (Color online) The intensity plots of the spectral functions as functions of the momentum and energy in the [(a) and (b)] SC state and [(c) and (d)] normal state, respectively. The left and right panels are along $(\pi, 0)$ to (π, π) , and $(0, 0)$ to (π, π) directions, respectively. The solid and dotted lines are the MDC dispersions and the bare band dispersions, respectively.

$= 10$ meV. The origin of the resonance has been studied intensively.^{30,31} It arises from a collective spin excitation mode corresponding to the real part of the RPA factor $(1 + U_{\mathbf{Q}} \text{Re} \chi_0)$ equals to zero and the imaginary part of the bare spin susceptibility $\text{Im} \chi_0$ is small. The resonance is absent in the normal state, where the peak intensity decreases dramatically and only a low-energy broad peak can be seen. While in fact the weight of the spectra are at low energies, and near AF momentum both in the SC and normal states.

Figures 2(a)–2(d) show the intensity maps of the spectral functions $[A(\mathbf{k}, \omega)f(\omega)]$ [$f(\omega)$ is the Fermi distribution function] as well as the MDC dispersions in the SC (up panels) and normal states (down panels), respectively. Clear kinks at the energy about $\omega_k \approx 60$ – 70 meV can be seen along the antinodal direction. Well defined quasiparticle peaks exist below the kink energy. At higher energy, the peak intensity is small. In the normal state the dispersion kink still exists and no qualitative difference can be seen.

The right panels of Fig. 2 show the nodal data of the spectral function. Here, the dispersion kink can also be seen clearly at the energy about $\omega_k = 60$ meV. The renormalized effect is much weaker than that of antinodal direction but does exist, which can be seen more clearly by comparing the dispersion with that of the bare band. As shown, the renormalized dispersion and the bare one are nearly parallel at high energies while the renormalized one bends to low energy at about 60 meV indicating that the kink is indeed caused by the self-energy. In addition, the peak intensity is larger at low energies ($\omega \leq \omega_k$), and decreases evidently at the kink energy. Similar with the case of antinodal direction, there is also no remarkable difference between the spectrum of the SC state with that of the normal state along the nodal direction.

The EDC line shapes along the antinodal and nodal directions are plotted in Fig. 3. Along the antinodal direction a sharp quasiparticle peak can be seen near the Fermi momen-

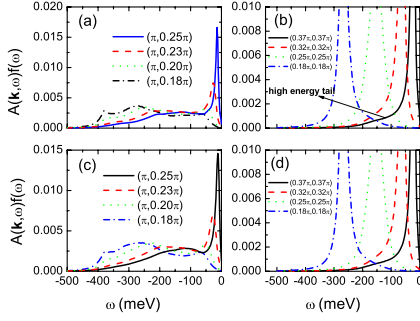


FIG. 3. (Color online) The line shape $A(\mathbf{k}, \omega)f(\omega)$ as a function of the energy at different momenta in the [(a) and (b)] SC state and [(c) and (d)] normal state, respectively. The left and right panels are along $(\pi, 0)$ to (π, π) , and $(0, 0)$ to (π, π) directions, respectively.

tum K_F following a 50 meV dip, which is consistent with the experiment as we mentioned above.¹⁸ The peak intensity decreases dramatically as the momentum is far away from K_F . Only a broad peak can be seen at the momentum $(\pi, 0.18\pi)$. Much weaker renormalized effect is obtained along the nodal direction, namely, a sharp quasiparticle peak accompanied by a high-energy humplike tail near the Fermi energy. At higher energies ($\omega \geq \omega_k$), the peak becomes a little broader while it is still well defined and the humplike tail disappears. The curve seems to be symmetric with respect to the peak energy. We can also see that there is no qualitative difference of the line shape between the SC and normal states.

Our theoretical results reproduce the dispersion kink. These results are qualitatively consistent with the experimental results^{17–20} although the nodal kink seems to be weaker than the experimental observations. Although the spin susceptibility shows remarkable difference between the SC and normal states, namely, a sharp resonance peak can be observed only in the SC state, as seen in Fig. 1, while the renormalized spectral function show no evident difference between the SC state and normal state. Although here we propose that the spin excitations should be responsible for the kink while in fact the spin-resonance phenomenon is not essential to the kink. In the following we demonstrate the origin of the kink and propose that the bare band structure and the renormalization by the spin susceptibility are both important to produce the kink.

A sound explanation for the dispersion kink can be given through analyzing the self-energy. The peak position is determined by the pole condition $\omega - \varepsilon_{\mathbf{k}} - \text{Re}\Sigma(\mathbf{k}, \omega) = 0$ in the normal state. The real part of the self-energy is responsible for the kink. Performing the summation over $i\omega_m$ [Eq. (5)], we can rewrite the self-energy as

$$\Sigma(\mathbf{k}, \omega) = \frac{1}{\pi N} \sum_{\mathbf{q}} \int g^2 \text{Im} \chi(\mathbf{q}, \omega_1) \frac{b(\omega_1) + 1 - f(\varepsilon_{\mathbf{k}-\mathbf{q}})}{\omega - \omega_1 - \varepsilon_{\mathbf{k}-\mathbf{q}} + i\delta} d\omega_1, \quad (8)$$

where $b(\omega)$ is the Bose distribution function. The real part of the self-energy is calculated by using the parameters of the bare band. The summation over $\sum_{\mathbf{q}}$ can be written as the integral form, $1/(\pi N) \sum_{\mathbf{q}} \rightarrow 4\pi \int d\mathbf{q} \rightarrow 4\pi \int d\varepsilon_{\mathbf{k}-\mathbf{q}} / [d\varepsilon_{\mathbf{k}-\mathbf{q}}/d\mathbf{q}]$.

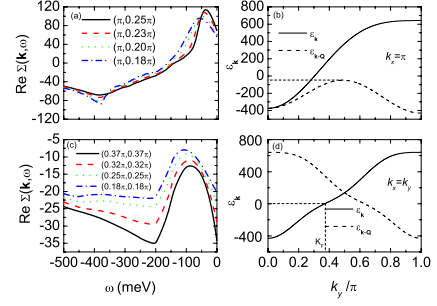


FIG. 4. (Color online) The real parts of the self-energies $\text{Re} \Sigma(\mathbf{k}, \omega)$ vs. the energy ω at different momenta and the bare band dispersions $\varepsilon_{\mathbf{k}}$ and $\varepsilon_{\mathbf{k}-\mathbf{Q}}$ along the [(a) and (b)] antinodal and [(c) and (d)] nodal directions, respectively.

The spin susceptibility is peaked at the AF momentum \mathbf{Q} and very low energy. As a result, approximately, the absolute of self-energy $|\Sigma|$ should have the maxima value and a kink is expected near the flat band, namely, $\nabla_{\mathbf{k}} \varepsilon_{\mathbf{k}-\mathbf{Q}} = 0$.

We show the real parts of the self-energies in the normal state and the bare band dispersions along the antinodal direction in Figs. 4(a) and 4(b). As seen in Fig. 4(a), the absolute values of the real part of the self-energy $|\text{Re} \Sigma|$ reach the local maximum at the energies about 50 and 400 meV. The origin of the two peaks can be seen from Fig. 4(b), namely, the band dispersion is flat ($\nabla_{\mathbf{k}} \varepsilon_{\mathbf{k}-\mathbf{Q}} = 0$) at the energies about 50 and 400 meV. As a result, the MDC dispersion has an obvious kink at the energies about 50–60 meV along the antinodal direction. The kink is always there, regardless $\text{Im} \chi(\mathbf{Q}, \omega)$ has a resonance peak or not (see Fig. 1).

The real parts of the self-energies and the bare band dispersions along nodal directions are shown in Figs. 4(c) and 4(d). As seen from Fig. 4(d), below the Fermi momentum $k < K_F$, $\varepsilon_{\mathbf{k}-\mathbf{Q}}$ is always greater than zero so that for negative energies the self-energy is quite small. Moreover, different from that along antinodal direction, there is in fact no obvious peak at low energies and the absolute value of $\text{Re} \Sigma$ is maximum at zero energy, indicating that the renormalized effect for peak position is prominent at low energies, consistent with the dispersion shown in Fig. 2. As the momentum is away from the Fermi momentum, the self-energy tends to be a constant at high energies so that the renormalized dispersion is parallel to the bare one at high energies, which can be seen in Fig. 2.

For the case of the SC state, because the SC gap is much less than the kink energy, the spin susceptibility is still peaked at very low energy. Thus in fact the SC gap does not influence the kink very much. We have also check numerously for different gap symmetry, i.e., the nonmonotonic d -wave gap¹⁵ and obtain similar results.

We now turn to address the renormalized effect of the density of states $[\rho(\omega) = fA(\mathbf{k}, \omega)d\mathbf{k}]$ in the SC state. Figure 5 shows the density of states as a function of the energy. The SC coherence peaks at the energies $\pm \Delta_0$ can be seen clearly. Outside the gaps the humplike features exist, and this reveals the existence of the bosonic mode, which is sensitive to the intensity and energy of the spin-resonance peak, and located at the energies about $\pm(\Delta_0 + \Omega_r)$ with $\Omega_r \sim 10$ meV; thus the spin-resonance mode should account for the humps outside

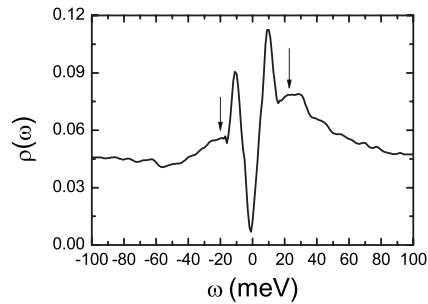


FIG. 5. The density of state as a function of the energy in the SC state.

the gap. This result is consistent with recent STM experiments on electron-doped cuprates.²¹ In hole-doped cuprates similar renormalized effect caused by the bosonic mode was also predicted theoretically³² and observed by STM experiments very recently.^{9–11} We can also see that the renormalized effect in the electron (negative energy) and hole parts (positive energy) is asymmetric. The intensity of the SC coherent peak is smaller and the renormalized hump caused by the spin resonance is also weaker at the negative-energy part.

In fact, the ARPES experiments can only examine the electronic structure in the electron part so that the possible renormalized effect at the energy $\Delta_0 + \Omega_r$ for spectral function $A(\mathbf{k}, \omega)$ is hard to detect and also is not obtained by our calculation. In fact, very recently the kink at about the energy 20 meV along nodal direction was reported by Ref. 20 while this result was not reported by other groups.^{17–19}

In summary, we study theoretically the effect of the spin-fluctuation mode on the spectral function and density of states in electron-doped cuprates. We have elaborated that the spin excitation is able to cause the 50–70 meV dispersion anomaly and the hump-like feature of density of states observed by recent experiments. Although here we still cannot rule out the contribution of other possible interactions, such as the phonon, while our results agree with the experiments qualitatively. Moreover we present a consistent picture of the effect of bosonic mode coupling for ARPES and STM spectra in electron-doped cuprates.

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¹For a review, see, e.g., P. A. Lee, N. Nagaosa, and X. G. Wen, *Rev. Mod. Phys.* **78**, 17 (2006).

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