Impurity effects on quasiparticle dispersion in a *d*-wave superconductor

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The effects of nonmagnetic impurity on the renormalization of quasiparticle (QP) dispersion in a $d_{x^2-y^2}$-wave superconductor are investigated theoretically using the self-consistent *t*-matrix approximation. It is shown that the kink in the dispersion around the antinodal region is weakened and disappears eventually with the increase in impurity concentration. In the meantime, the dip in the peak/dip/hump structure of the QP line shape is smeared out and the peak is suppressed and broadened upon the introduction of impurities. We attribute these effects to the suppression and broadening of the spin-resonance mode by impurity, which is coupled strongly to quasiparticles. These results are consistent qualitatively with the recent experiments and give support to the scenario that the quasiparticle renormalization around the antinodal region is mainly of magnetic origin.

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I. INTRODUCTION

For decades, copper oxide superconductors with high transition temperature have been studied intensively. Angle-resolved photoemission spectroscopy (ARPES) can provide direct information of quasiparticle (QP) dispersion, from which we may study the driving force of high-T_c superconductors (HTSCs). It has been revealed by ARPES that there exists a peak/dip/hump (PDH) structure in the QP spectral line shape.[1,2] After disentangling bilayer splitting, the PDH structure is seen around the $(\pi,0)$ point in both the bonding and antibonding bands.[3–5] Besides, another interesting feature is the unusual segment in the QP dispersion, the so-called "kink," which has been found both around the nodal and antinodal regions of the Brillouin zone (BZ).[3–10] The kinks in the QP dispersion reflect the renormalization effect of interactions on quasiparticles with its strength relating to the coupling strength and its energy scale to the coupling mode energy. Different from the nodal direction, kinks in the antinodal region occur only in the superconducting state with a stronger strength, lower energy scale, and more prominent temperature dependence.[4]

Impurity scattering is a common effect and can be used to probe the physical properties of a superconductor. For copper oxide superconductors, Zn and Ni are the usually used impurity elements since they have almost the same atomic mass as Cu but different spin states. Substitution by Zn (or Ni) for Cu changes the magnetic environment while preserving the carrier concentration and introducing little change to the lattice structure. This can be regarded as the magnetic "isotope" effect. According to Anderson's theorem, the transition temperature and superconducting gap are not sensitive to nonmagnetic impurities in *s*-wave superconductors, while for *d*-wave superconductors, nonmagnetic impurities are pair breakers. When copper ions in the Cu-O plane of a *d*-wave superconductor are substituted by nonmagnetic impurity ions, such as Zn^{2+}, the superconducting transition temperature will be rapidly suppressed.[11]

In the vicinity of the $(\pi,0)$ point of the BZ, the superconducting gap and the pairing correlation reach their maximum, so the anomalies of the QP line shape here are supposed to be important for the understanding of the mechanism of HTSCs. It is widely believed that the coupling to a collective bosonic mode will naturally interpret these anomalies.[12,13] Mainly, two kinds of modes have been proposed to account for the $(\pi,0)$ kink, the phonon, and the spin-resonance modes, but which one dominates is still under debate.[3–9] A spin-resonance mode with a sharp peak centered at the antiferromagnetic (AF) wave vector (π,π) is observed in inelastic neutron-scattering (INS) experiments in the superconducting and the pseudogap states.[14–17] When the momentum moves away from the AF wave vector, the intensity of the resonance peak decreases promptly. Several ARPES studies on the QP dispersion have suggested an intimate relationship between the features in the spectral line shape[3,4,7,18] and the spin-resonance mode, and therefore have stimulated many theoretical studies.[19–22]

Recent ARPES experiments show that the kink strength in the QP dispersion around the antinodal region is markedly weakened by nonmagnetic impurities.[23,24] Also the coupling strength is reduced by nonmagnetic impurities. In the meantime, the dip in the peak/dip/hump structure of the QP line shape is smeared out upon the introduction of impurities.[25] On the other hand, the INS experiments show that zinc ions in the Cu-O planes produce large modifications to the spin susceptibility.[26,27] In view of these experimental data, we will here study the effects of impurities on the QP dispersion based on the spin-resonance scenario. We start our study with a bilayer $d_{x^2-y^2}$-wave superconductor with nonmagnetic impurities. Impurities are considered in the dilute and unitary limit, with the self-consistent *t*-matrix approximation.[28–30] We find that the kink structure in the QP dispersion of the bonding band around the antinodal region is weakened and disappears eventually with the increase in impurity concentration. While in the nodal region, no kink structure appears and a little effect of the impurity on the dispersion is detected. The PDH structure of the bonding band spectra is modified greatly by nonmagnetic impurities, while the antibonding band is changed slightly. The peak is suppressed, broadened, and shifted to lower frequencies upon the introduction of nonmagnetic impurities. On the other hand, the dip is broadened and smeared out progressively. These results are in good agreement with recent experiments.[23–25]

We organize this paper as follows. In Sec. II, we introduce the theoretical model and analytical calculation. In Sec. III, numerical calculations are carried out and the results are discussed. In Sec. IV, we make a concluding remark.

II. THEORY AND MODEL

In order to consider impurity effects, we start from the impurity-average Nambu Green's function for single particles in a bilayer superconductor,[28,31]

$$\hat{g}^{(i)}(\mathbf{k},i\omega_n)=\frac{i\tilde{\omega}_n^{(i)}\hat{\sigma}_0+\tilde{\Delta}_k\hat{\sigma}_1+\tilde{\xi}_k^{(i)}\hat{\sigma}_3}{(i\tilde{\omega}_n^{(i)})^2-\tilde{\Delta}_k^2-(\tilde{\xi}_k^{(i)})^2}, \tag{1}$$

where $\hat{\sigma}_j(\hat{\sigma}_0=\hat{\mathbf{1}})$ are the Pauli matrices and the upper index $i=a$ or b represents the antibonding or bonding band. The tilde symbol indicates the inclusion of impurity-scattering self-energy corrections,

$$\tilde{\omega}_n^{(i)}=\omega_n-\Sigma_0^{(i)}(\omega_n),$$

$$\tilde{\Delta}_k=\Delta_k+\Sigma_1^{(i)}(\omega_n),$$

$$\tilde{\xi}_k^{(i)}=\xi_k^{(i)}+\Sigma_3^{(i)}(\omega_n). \tag{2}$$

For the quasiparticle dispersion, we use $\xi_k^{(a/b)}=-2t(\cos k_x+\cos k_y)-4t'\cos k_x\cos k_y-2t''[\cos(2k_x)+\cos(2k_y)]-\mu\pm t_\perp$, with $t'/t=-0.2$, $t''/t=0.25$, $t_\perp/t=0.44$, and $\mu/t=-1.11$, corresponding to a fit to the ARPES data on optimal doping yttrium barium copper oxide (YBCO) as used before,[32,33] in which t is taken to be 115 meV. The superconducting gap function is taken as $\Delta_k=\Delta_0(\cos k_x-\cos k_y)/2$, where $\Delta_0=4T_{c0}$; T_{c0} is the SC transition temperature. In the following calculations, all parameters are in unit of t. For a d-wave gap, the correction to the gap function Σ_1 vanishes. We neglect the interactions between impurities and take the single-site approximation, then the impurity self-energy will be given by $\Sigma_j^{(i)}=\Gamma T_j^{(i)}$, with $\Gamma=n_i/\pi N_0$, where N_0 is the normal phase density of states and n_i is the impurity concentration. The impurity-scattering t-matrix $T_j^{(i)}$ can be calculated from[28,31]

$$T_0^{(i)}=\frac{G_0^{(i)}(\omega)}{c^2-[G_0^{(i)}(\omega)]^2},\quad T_3^{(i)}=\frac{-c}{c^2-[G_0^{(i)}(\omega)]^2}, \tag{3}$$

with $G_0^{(i)}(\omega)=(1/\pi N_0)\Sigma_k\mathrm{Tr}[\hat{\sigma}_0\hat{g}^{(i)}(\mathbf{k},\omega)]$. Here $c=\cot\delta_0$ and δ_0 is the scattering phase shift. In the unitary limit, $c=0$, so only the contribution from Σ_0 remains. In the presence of impurities, the superconducting energy gap $\Delta(\Gamma,0)$ and the transition temperature T_c need to be determined from the gap equation. In the weak-coupling limit, it has been found that $\Delta(\Gamma,0)/\Delta_0\approx T_c/T_{c0}$.[30] The temperature-dependent energy gap $\Delta(\Gamma,T)$ is

$$\Delta(\Gamma,T)=\Delta(\Gamma,0)\tanh[2\sqrt{(T_c/T)-1}], \tag{4}$$

where T_c is given by the Abrikosov-Gor'kov formula,[34]

$$-\ln\left(\frac{T_c}{T_{c0}}\right)=\psi\left(\frac{1}{2}+\frac{\Gamma}{2\pi T_c}\right)-\psi\left(\frac{1}{2}\right), \tag{5}$$

with $\psi(x)$ the digamma function. The spin susceptibility with Matsubara frequency is

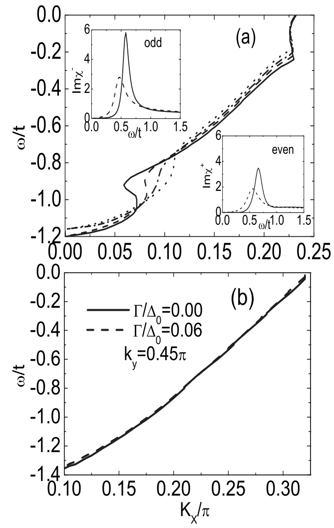

FIG. 1. (a) Bonding band MDC dispersion of quasiparticles in the antinodal region ($k_y=\pi$) for different impurity concentrations; the solid line is for $\Gamma/\Delta_0=0$, the dashed line is for 0.02, and the dashed-dotted and dotted lines are for 0.04 and 0.06, respectively. The insets in (a) present the spin-resonance modes of the odd channel (χ^-) and even channel (χ^+) at (π,π) point, with the solid line for $\Gamma/\Delta_0=0$ and dashed line for $\Gamma/\Delta_0=0.06$. (b) Bonding band MDC dispersion in the nodal region.

$$\chi_0^{(ij)}(\mathbf{q},i\omega_m)=-\frac{T}{N}\sum_n\sum_{\mathbf{k}}\mathrm{Tr}\left[\frac{1}{2}\hat{g}^{(i)}(\mathbf{k},i\omega_n)\cdot\hat{g}^{(j)}(\mathbf{k}+\mathbf{q},i\omega_m+i\omega_n)\right]. \tag{6}$$

Using Padé approximants,[35] we will get its analytical continuation to the real frequency $\chi_0^{(ij)}(\mathbf{q},\omega)$. The physical spin susceptibility is given by $\chi=\chi_0^+\cos^2(q_zc/2)+\sin^2(q_zc/2)$, with $\chi_0^+=\chi^{aa}+\chi^{bb}$ and $\chi_0^-=\chi^{ab}+\chi^{ba}$. We include the spin-fluctuation effect through the random-phase approximation (RPA),[36] in which the renormalized spin susceptibility is

$$\chi^{\pm}(\mathbf{q},\omega)=\frac{\chi_0^{\pm}(\mathbf{q},\omega)}{1+(J_{\mathbf{q}}\pm J_\perp)\chi_0^{\pm}(\mathbf{q},\omega)}. \tag{7}$$

Here we take the RPA correction factor $J_{\mathbf{q}}=J[\cos(q_x)+\cos(q_y)]$. We take $J=0.9$ so that the peak of the spin resonance in the odd channel for the pristine system is at $E_r=60$ meV [see the inset of Fig. 1(a)]. This value is slightly larger than the experimental data which is at 41–55 meV.[14,37] To get a lower E_r, one needs to increase J, but this does not qualitatively change the results we present in the following. The interlayer exchange integral $J_\perp$ is taken as 0.1. The fermionic self-energy coming from the coupling of electrons to the spin-resonance mode is

$$\Sigma_{s,w}^{(a,b)}(\mathbf{k})=\pm\frac{T}{N}\sum_{\mathbf{q}}[(J_{\mathbf{q}}+J_\perp)^2\chi^+(\mathbf{q})\mathcal{G}_{s,w}^{(a,b)}(\mathbf{k}-\mathbf{q})+(J_{\mathbf{q}}-J_\perp)^2\chi^-(\mathbf{q})\mathcal{G}_{s,w}^{(b,a)}(\mathbf{k}-\mathbf{q})], \tag{8}$$

where the + (−) denotes the normal (abnormal) self-energy

$\Sigma_{s(w)}$ and the symbol $\mathbf{q}$ is an abbreviation of $(\mathbf{q},i\omega_m)$. $\mathcal{G}_s$ ($\mathcal{G}_w$) is the bare normal (abnormal) Green's function of superconducting electrons, with $\mathcal{G}_s=\hat{g}_{11}$ and $\mathcal{G}_w=\hat{g}_{12}$.

Finally, we get the renormalized Green's function,

$$G^{(a,b)}(\mathbf{k},i\omega)=\{[G_s^{(a,b)}(\mathbf{k},i\omega)]^{-1} + (\Delta_{\mathbf{k}}+\Sigma_w^{(a,b)})^2 G_s^{(a,b)}(\mathbf{k},-i\omega)\}^{-1}, \qquad (9)$$

with $G_s^{(a,b)}=[i\omega-\xi^{(a,b)}-\Sigma_s^{(a,b)}]^{-1}$. The spectral function is given by $A(\mathbf{k},\omega)=-(1/\pi)\mathrm{Im}[G(\mathbf{k},\omega+i\delta)]$.

Numerical calculations are carried out on a 64×64 lattice at a temperature $T=0.1T_{c0}$, with $T_{c0}=0.1$. Equations (1)–(3) form a closed set of equations and will be solved self-consistently in the imaginary frequencies to get the renormalized Green's function. Then the spin susceptibility is calculated with this Matsubara Green's function. The analytical continuation of the spin susceptibility is performed using Padé approximants.

III. RESULTS AND DISCUSSION

In Fig. 1(a), we show the quasiparticle dispersion obtained from the momentum distribution curve (MDC) of the bonding band around the antinodal region for the pristine case (solid line) and those with several impurity concentrations. The so-called MDC corresponds to the plot of $A(\mathbf{k},\omega)$ versus $\mathbf{k}$, with ω fixed and the renormalized dispersion is given by the peak position of the MDC. For the pristine case, an obvious kink in the renormalized energy band is observed starting from $0.85t$. With the increase in the impurity concentration, the energy at which the kink occurs decreases and in the meantime the kink structure becomes weaker. At the largest impurity concentration considered here $\Gamma/\Delta_0=0.06$, the kink is almost removed. Interestingly, in this process, the quasiparticle dispersion does not show qualitative change with impurity concentration both above and below the kink region. A quantitative change exhibiting the shift of the energy band to lower binding energy as a whole is observed, which results from the reduction in the magnitude of the superconducting gap upon the introduction of impurities. These results are consistent with the recent ARPES experiments.[23,24] As for the antibonding band, we find that it is less affected by the coupling to the spin fluctuation and no kink is detected. There are two reasons for this difference. (i) The self-energy [Eq. (8)] has a feature that the quasiparticles in the bonding (antibonding) band are scattered into the antibonding (bonding) band via the spin fluctuation in the odd channel χ^- in which the strong spin resonance is observed [see the insets of Fig. 1(a)]. (ii) The antibonding band and its associated flat band near the antinodal region are much closer to the Fermi surface compared to the bonding band. As a result, the bonding band is more strongly renormalized than the antibonding band.

Figure 1(b) shows the quasiparticle dispersion of the bonding band around the nodal region. In this case, no kink structure is observed even for the pristine system. Correspondingly, a little effect of the impurity on the dispersion appears. We note that a similar kink structure has also been observed around the nodal region by ARPES

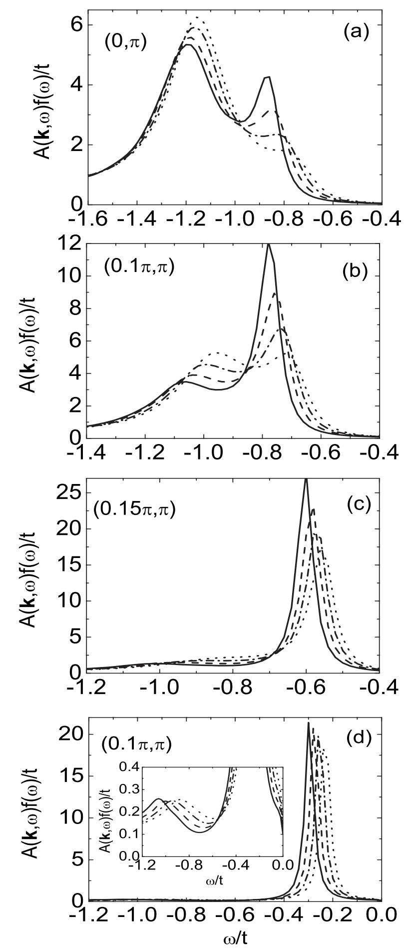

FIG. 2. (a)–(c) are bonding band spectra $A(\mathbf{k},\omega)f(\omega)$ at $k=(0,\pi),(0.1\pi,\pi),(0.15\pi,\pi)$ for various impurity concentrations. (d) is for the antiboding band at $(0.1\pi,\pi)$ point of the BZ. The inset in (d) shows the fine structure of the PDH line shape of the antibonding band at $(0.1\pi,\pi)$ point. The solid line is for $\Gamma/\Delta_0=0$, the dashed line is for 0.02, and the dashed-dotted and dotted lines are for 0.04 and 0.06, respectively.

measurements.[6,8] However, its temperature, momentum, and doping dependences suggest that it may not be of magnetic origin but of phonon or other origins. Simply from the transferred momentum, one will expect that the spin resonance contributes little to the node-to-node scattering because the transferred momentum is much less than (π,π) at which the spin resonance appears. Therefore, we cannot reproduce the observed kink structure in the current model in which only the coupling of quasiparticles to spin fluctuations is considered.

A related feature in the quasiparticle line shape is the peak/dip/hump structure. In Figs. 2(a)–2(c) the line shape $A(\mathbf{k},\omega)f(\omega)$ [$f(\omega)$ is the Fermi distribution function] in the bonding band for different k points is presented. Let us first discuss the case without impurity. Near the kink energy, an obvious peak/dip/hump structure can be observed. From $(0,\pi)$ to the nodal region, the intensity of the quasiparticle peak increases rapidly, while the hump and consequently the dip become weak. So, near the nodal region, this structure disappears completely. When the binding energy is below the kink energy, the intensity of the peak in the peak/dip/hump structure is larger than that of the hump, while it is smaller than the hump when the binding energy is above the kink energy. In the dispersion shown in Fig. 1(a), this behavior is exhibited as two sections of the renormalized dispersions connected by the kink. Therefore, the appearance of the kink in the dispersion involves the crossover from the stronger peak intensity to stronger hump intensity when binding energy is increased [see Figs. 2(a) and 2(b)]. With impurities, the quasiparticle peak is suppressed and broadened gradually. Its peak position is also shifted slightly to lower binding energy. For the k points below the kink position, such as shown in Fig. 2(c), the dip is smeared out completely at the impurity concentration $\Gamma/\Delta_0=0.04$. Therefore, no peak/dip/hump structure exists anymore. When the k point moves toward the $(0,\pi)$ point, the effect of the impurity on the peak/dip/hump structure is to enhance the hump associated with the depression of the quasiparticle peak. Therefore, the peak/dip/hump structure also disappears as the quasiparticle peak is removed completely by the impurity at $\Gamma/\Delta_0=0.06$. These qualitative effects of the impurity on the peak/dip/hump structure agree with the ARPES experiment.[24,25] In Fig. 2(d), we also show the line shape of quasiparticles in the antibonding band. A faint peak/dip/hump structure may be detected and it is less affected by the impurity [see the inset of Fig. 2(d)], except that the quasiparticle peak is suppressed and broadened.

Due to the coupling to spin fluctuations, the quasiparticle dispersion is renormalized. As shown in the insets of Fig. 1(a), the sharp spin-resonance modes exist in the spectrum of spin fluctuations, in particular in the odd channel. For the pristine case, this sharp mode will lead to a steplike rise in the imaginary part of the quasiparticle self-energy $\mathrm{Im}\,\Sigma(\omega)$ with its peak at the frequency $E_r+\Delta_0\sim 0.94t$ [E_r is the mode energy and Δ_0 is the superconducting gap at $(0,\pi)$; see Fig. 3(a)] and consequently a logarithmic divergence (exhibiting a peak due to the finite lattice size and the lifetime effect) in its real part as shown in Fig. 3(b).[22] This divergence gives rise to a strong renormalization to the quasiparticle dispersion exhibiting a kink structure. In the meantime, it leads to the dip in the quasiparticle line shape. Physically, this amounts to the fact that the quasiparticle acquires a decaying channel provided by the spin resonance when its energy matches the excitation energy of the spin-resonance mode plus the quasiparticle excitation energy across the superconducting gap. With impurities, the steplike rise and the divergency (the peak) are suppressed; therefore it weakens and eventually smears out the kink in the dispersion and the dip in the line shape. This suppression stems from the effect of the impurity on the spin resonance. As shown in the insets of Fig. 1(a), the spin-resonance peak is suppressed, broadened, and shifted to lower frequencies upon impurity introduction, which is consistent with the result obtained before.[32] Therefore, the weakening of the dispersion kinks and the smearing out of the dip are essentially due to the effect of the impurity on the spin resonance and in turn on the quasiparticle self-energy. We note that, as discussed above, it is the relative intensity between the peak and hump, which affects the kink structure. Thus, though the numerical changes in the self-energy [shown in Figs. 3(a) and 3(b)] are not so large, they

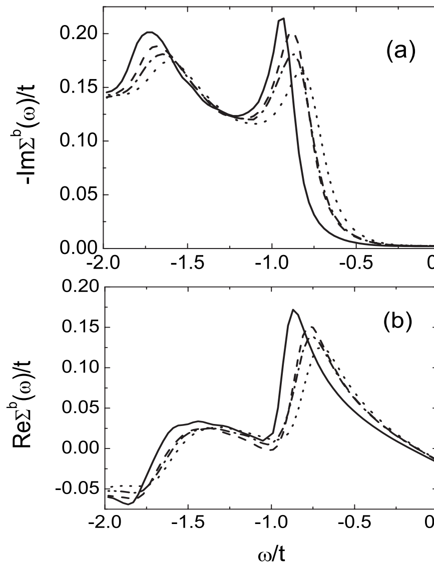

FIG. 3. Imaginary and real parts of the bonding band self-energy versus frequency ω for various impurity concentrations Γ/Δ_0 at the $(0,\pi)$ point. The solid line is for $\Gamma/\Delta_0=0$, the dashed line is for 0.02, and the dashed-dotted and dotted lines are for 0.04 and 0.06, respectively.

affect the relative intensity effectively. As for the second peak (hump) in the self-energy as shown in Fig. 3, we notice that Eq. (8) shows that the self-energy in the bonding band is composed of two parts: the coupling of bonding band quasiparticles to the even channel spin-resonance mode and the coupling of antibonding band quasiparticles to the odd channel spin-resonance mode. The former coupling will lead to a peak (hump) at energy $\Omega^{+}+E^{b}$, with Ω^{+} as the even channel mode energy and E^{b} the bare quasiparticle energy in the bonding band.

Finally, we note that the nonmagnetic impurity in high-T_c superconductors will also induce a local magnetic moment and give rise to an additional spin-flip scattering effect. The origin of the induced magnetic moment is still under investigation and not reproduced in our study. Therefore, an additional effect from this feature is unclear and will wait for the future study.

IV. CONCLUSION

We have studied the quasiparticle dispersion and the spectral line shape in a bilayer d-wave superconductor with nonmagnetic impurities. The renormalization of the quasiparticle energy band is assumed to be scattered off the spin-resonance mode in the spin excitation spectrum. Without impurity, a clear kink in the quasiparticle dispersion and a peak/dip/hump structure in the line shape are presented near the antinodal region. When the impurity is introduced, we find that the kink is weakened gradually and eventually disappears. In the meantime, the dip in the peak/dip/hump structure is smeared out gradually and the quasiparticle peak is suppressed, broadened, and shifted to lower frequencies. These qualitative features are consistent with recent ARPES experiments. The origin of these features is attributed to the suppression and the broadening of the spin-resonance mode. Therefore, our investigation gives support to the scenario that the quasiparticle renormalization around the antinodal region is mainly due to the coupling to spin fluctuations.

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