Out-of-plane impurities induce deviations from the monotonic *d*-wave superconducting gap of cuprate superconductors

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The electronic structure of cuprate superconductors is studied within the kinetic-energy-driven superconducting mechanism in the presence of *out-of-plane impurities*. With increasing impurity concentration, although both superconducting coherence peaks around the nodal and antinodal regions are suppressed, the position of the leading-edge midpoint of the electron spectrum around the nodal region remains at the same position, whereas around the antinodal region it is shifted toward higher binding energies, this leads to a strong deviation from the monotonic *d*-wave superconducting gap in the out-of-plane impurity-controlled cuprate superconductors.

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I. INTRODUCTION

The superconducting gap is a fundamental property of superconductors,[1] and the nature of its anisotropy has played a crucial role in the testing of the microscopic theory of superconductivity in cuprate superconductors.[2] Experimentally, by virtue of systematic measurements,[3] particularly using the angle-resolved photoemission spectroscopy (ARPES) technique,[4] the *d*-wave nature of the superconducting gap has been well established by now. In particular, this *d*-wave superconducting symmetry remains one of the cornerstones of our understanding of the physics in cuprate superconductors.[3–7] The early ARPES measurements on the cuprate superconductor $Bi_2Sr_2CaCu_2O_{8+\delta}$ (Ref. 8) showed that in the real space the gap function and the pairing force have a range of one lattice spacing, and then the superconducting-gap function is of the monotonic *d*-wave form $\Delta_{\mathbf{k}}=\Delta[\cos k_x-\cos k_y]/2$. Later, the ARPES measurements on the cuprate superconductor $Bi_2Sr_2CaCu_2O_{8+\delta}$ (Ref. 9) indicated that the superconducting gap significantly deviates from this monotonic *d*-wave form. Furthermore, it was argued that this deviation should be attributed to an increase in the electron correlation, which may increase the intensity of the higher order of the harmonic component in the monotonic *d*-wave gap function.[9] However, recent ARPES measurements[10,11] on the cuprate superconductors $(Bi,Pb)_2(Sr,La)_2CuO_{6+\delta}$ and $Bi_2Sr_{1.6}Ln_{0.4}CuO_{6+\delta}$ (*Ln*-Bi2201) with *Ln*=La, Nd, and Gd showed that a much stronger deviation from the monotonic *d*-wave superconducting-gap form is unlikely to be due to the strong correlation effect.

The cuprate superconductors have a layered structure consisting of the two-dimensional CuO_2 layers separated by insulating layers.[12,13] The single common feature is the presence of the CuO_2 plane,[4,13] and it seems evident that the unusual behaviors of cuprate superconductors are dominated by this CuO_2 plane.[2] It has been well established that the Cu^{2+} ions exhibit an antiferromagnetic long-range order in the parent compounds of cuprate superconductors, and superconductivity occurs when the antiferromagnetic long-range order state is suppressed by doped charge carriers.[13] Since these doped charge carriers are induced by the replacement of ions by those with different valences or the addition of excess oxygens in the block layer, therefore in principle, all cuprate superconductors have naturally impurities (or disorder). However, for the cuprate superconductors $(Bi,Pb)_2(Sr,La)_2CuO_{6+\delta}$ and *Ln*-Bi2201, the mismatch in the ionic radius between Bi and Pb or Sr and *Ln* causes the *out-of-plane impurities*,[14] where the concentration of the out-of-plane impurities is controlled by varying the radius of the Pb or *Ln* ions, and then the superconducting transition temperature T_c is found to be decreasing with increasing impurity concentration. These cuprate superconductors $(Bi,Pb)_2(Sr,La)_2CuO_{6+\delta}$ and *Ln*-Bi2201 are often referred to as the out-of-plane impurity-controlled cuprate superconductors. Recently, the electronic structure of the out-of-plane impurity-controlled cuprate superconductors and the related superconducting-gap function have been investigated experimentally by using ARPES.[10,11] It was shown that although the effect of the out-of-plane impurity scattering around the antinodal region is much stronger than that around the nodal region, both superconducting coherence peaks around the nodal and antinodal regions are suppressed. Furthermore, the magnitude of the deviation from the monotonic *d*-wave superconducting-gap form increases with increasing impurity concentration.[10,11] The appearance of the strong deviation from the monotonic *d*-wave superconducting-gap form, observed recently in the out-of-plane impurity-controlled cuprate superconductors $(Bi,Pb)_2(Sr,La)_2CuO_{6+\delta}$ and *Ln*-Bi2201, is the most remarkable effect,[10,11] however, its full understanding is still a challenging issue. To the best of our knowledge, this strong deviation from the monotonic *d*-wave superconducting-gap form in the out-of-plane impurity-controlled cuprate superconductors has not been treated starting from a microscopic superconducting theory yet.

In the absence of out-of-plane impurity scattering, the electronic structure of cuprate superconductors in the superconducting state has been discussed[15,16] within the framework of the kinetic-energy-driven superconductivity,[17] where the superconducting-gap function has a monotonic *d*-wave form, and the main features of the ARPES experiments[4] on cuprate superconductors have been reproduced. In this paper, we study the electronic structure of the out-of-plane impurity-controlled cuprate superconductors in the superconducting state and the related superconducting-gap function along with this line. We employ the *t*-*J* model by considering the out-of-plane impurity scattering, and then show explicitly that the strong deviation from the monotonic *d*-wave superconducting-gap form occurs due to the presence of the impurity scattering. Although both sharp superconducting coherence peaks around the nodal and antinodal regions are suppressed, the effect of the impurity scattering is stronger in the antinodal region than that in the nodal region. Our results also show that the electronic structure of the out-of-plane impurity-controlled cuprate superconductors in the superconducting state can be understood within the framework of the kinetic-energy-driven superconducting mechanism with the out-of-plane impurity scattering taken into account.

This paper is organized as follows. In Sec. II we present the basic formalism of the electronic-structure calculation in the presence of the out-of-plane impurities. Within this theoretical framework, we discuss the electronic structure of the out-of-plane impurity-controlled cuprate superconductors in the superconducting state and the related superconducting-gap function in Sec. III, where we show that the well-pronounced deviation from the monotonic *d*-wave superconducting-gap form is mainly caused by the out-of-plane impurity scattering. Finally, we give a summary in Sec. IV.

II. FORMALISM

It has been shown that the essential physics of cuprate superconductors is properly accounted by the two-dimensional *t*-*J* model on a square lattice,[2]

$$H = -t\sum_{i\hat{\eta}\sigma} C^{\dagger}_{i\sigma}C_{i+\hat{\eta}\sigma} + t'\sum_{i\hat{\tau}\sigma} C^{\dagger}_{i\sigma}C_{i+\hat{\tau}\sigma} + \mu\sum_{i\sigma} C^{\dagger}_{i\sigma}C_{i\sigma} + J\sum_{i\hat{\eta}} \mathbf{S}_i\cdot\mathbf{S}_{i+\hat{\eta}}, \tag{1}$$

acting on the Hilbert subspace with no doubly occupied site, i.e., $\sum_\sigma C^{\dagger}_{i\sigma}C_{i\sigma}\leq 1$, where $\hat{\eta}=\pm\hat{x},\pm\hat{y}$, $\hat{\tau}=\pm\hat{x}\pm\hat{y}$, $C^{\dagger}_{i\sigma}$ ($C_{i\sigma}$) is the creation (annihilation) operator of an electron with spin σ, $\mathbf{S}_i=(S^x_i,S^y_i,S^z_i)$ are spin operators, and μ is the chemical potential. To deal with the constraint of no double occupancy in analytical calculations, the charge-spin separation fermion-spin theory[18] has been developed, where the constrained electron operators $C_{i\uparrow}$ and $C_{i\downarrow}$ are decoupled as $C_{i\uparrow}=h^{\dagger}_{i\uparrow}S^-_i$ and $C_{i\downarrow}=h^{\dagger}_{i\downarrow}S^+_i$, respectively, here the spinful fermion operator $h_{i\sigma}=e^{-i\Phi_{i\sigma}}h_i$ describes the charge degree of freedom together with some effects of spin configuration rearrangements due to the presence of the doped charge carrier itself, while the spin operator S_i describes the spin degree of freedom, then the electron on-site local constraint for the single occupancy, $\sum_\sigma C^{\dagger}_{i\sigma}C_{i\sigma}=S^+_ih_{i\uparrow}h^{\dagger}_{i\uparrow}S^-_i+S^-_ih_{i\downarrow}h^{\dagger}_{i\downarrow}S^+_i =h_ih^{\dagger}_i(S^+_iS^-_i+S^-_iS^+_i)=1-h^{\dagger}_ih_i\leq 1$, is satisfied in analytical calculations. In particular, it has been shown that under the decoupling scheme, this charge-spin separation fermion-spin representation is a natural representation of the constrained electron defined in the Hilbert subspace without double electron occupancy.[16] Furthermore, these charge carrier and spin are gauge invariant,[18] and in this sense they are real and can be interpreted as physical excitations.[19] In this charge-spin separation fermion-spin representation, the *t*-*J* model [Eq. (1)] can be expressed as,

$$H = t\sum_{i\hat{\eta}} (h^{\dagger}_{i+\hat{\eta}\uparrow}h_{i\uparrow}S^+_iS^-_{i+\hat{\eta}} + h^{\dagger}_{i+\hat{\eta}\downarrow}h_{i\downarrow}S^-_iS^+_{i+\hat{\eta}}) - t'\sum_{i\hat{\tau}} (h^{\dagger}_{i+\hat{\tau}\uparrow}h_{i\uparrow}S^+_iS^-_{i+\hat{\tau}} + h^{\dagger}_{i+\hat{\tau}\downarrow}h_{i\downarrow}S^-_iS^+_{i+\hat{\tau}}) - \mu\sum_{i\sigma} h^{\dagger}_{i\sigma}h_{i\sigma} + J_{\rm eff}\sum_{i\hat{\eta}} \mathbf{S}_i\cdot\mathbf{S}_{i+\hat{\eta}}, \tag{2}$$

with $J_{\rm eff}=(1-\delta)^2J$, and $\delta=\langle h^{\dagger}_{i\sigma}h_{i\sigma}\rangle=\langle h^{\dagger}_ih_i\rangle$ being the charge-carrier doping concentration. This $J_{\rm eff}$ is similar to that obtained in Gutzwiller approach.[7] As an important consequence, the kinetic-energy term in the *t*-*J* model has been transferred as the interaction between charge carriers and spins, which reflects that even the kinetic-energy term in the *t*-*J* Hamiltonian has a strong Coulombic contribution due to the restriction of no double occupancy of a given site. This interaction from the kinetic-energy term is quite strong, and it has been shown[17] in terms of the Eliashberg's strong coupling theory[20] that in the case without an antiferromagnetic long-range order, this interaction can induce a charge-carrier pairing state (then the electron Cooper pairing state) with *d*-wave symmetry by exchanging spin excitations in the higher power of the charge-carrier doping concentration δ. In this case, the electron Cooper pairs originating from the charge-carrier pairing state are due to the charge-spin recombination, and their condensation reveals the *d*-wave superconducting ground state. Furthermore, this *d*-wave superconducting state is controlled by both the superconducting-gap function and the quasiparticle coherence, which leads to the fact that the maximal superconducting transition temperature occurs around the optimal doping, and then decreases in both underdoped and overdoped regimes.[17] Moreover, it has been shown[15,16] that this superconducting state is the conventional Bardeen-Cooper-Schrieffer (BCS) like[1,21] with the *d*-wave symmetry, so that the basic BCS formalism with the *d*-wave superconducting-gap function is still valid in quantitatively reproducing all main low-energy features of the ARPES experimental measurements on cuprate superconductors, although the pairing mechanism is driven by the kinetic energy by exchanging spin excitations, and other exotic magnetic scattering[22] is beyond the BCS formalism. Following previous discussions,[15–17] the full charge-carrier Green's function in the superconducting state with a monotonic *d*-wave gap function can be obtained in the Nambu representation as,[23]

$$\tilde{g}(\mathbf{k},\omega) = Z_{hF}\frac{1}{\omega^2-E^2_{h\mathbf{k}}}\begin{pmatrix}\omega+\bar{\xi}_{\mathbf{k}} & \bar{\Delta}_{hZ}(\mathbf{k})\\ \bar{\Delta}_{hZ}(\mathbf{k}) & \omega-\bar{\xi}_{\mathbf{k}}\end{pmatrix} = Z_{hF}\frac{\omega\tau_0+\bar{\Delta}_{hZ}(\mathbf{k})\tau_1+\bar{\xi}_{\mathbf{k}}\tau_3}{\omega^2-E^2_{h\mathbf{k}}}, \tag{3}$$

where τ_0 is the unit matrix, τ_1 and τ_3 are the Pauli matrices, the renormalized charge-carrier excitation spectrum $\bar{\xi}_{\mathbf{k}}=Z_{hF}\xi_{\mathbf{k}}$, with the mean-field charge-carrier excitation spectrum $\xi_{\mathbf{k}}=Zt\chi_1\gamma_{\mathbf{k}}-Zt'\chi_2\gamma'_{\mathbf{k}}-\mu$, the spin-correlation functions $\chi_1=\langle S_i^+S_{i+\hat{\eta}}^-\rangle$ and $\chi_2=\langle S_i^+S_{i+\hat{\tau}}^-\rangle$, $\gamma_{\mathbf{k}}=(1/Z)\Sigma_{\hat{\eta}}e^{i\mathbf{k}\cdot\hat{\eta}}$, $\gamma'_{\mathbf{k}}=(1/Z)\Sigma_{\hat{\tau}}e^{i\mathbf{k}\cdot\hat{\tau}}$, Z is the number of the nearest-neighbor or next-nearest-neighbor sites, the renormalized charge-carrier monotonic d-wave pair gap function $\bar{\Delta}_{hZ}(\mathbf{k})=Z_{hF}\bar{\Delta}_h(\mathbf{k})$, where the effective charge-carrier monotonic d-wave pair gap function $\bar{\Delta}_h(\mathbf{k})=\bar{\Delta}_h\gamma_{\mathbf{k}}^{(d)}$ with $\gamma_{\mathbf{k}}^{(d)}=(\cos k_x-\cos k_y)/2$, and the charge-carrier quasiparticle spectrum $E_{h\mathbf{k}}=\sqrt{\bar{\xi}_{\mathbf{k}}^2+|\bar{\Delta}_{hZ}(\mathbf{k})|^2}$. The charge-carrier quasiparticle coherent weight Z_{hF} and effective charge-carrier gap parameter $\bar{\Delta}_h$ are determined by the following two equations:[15–17]

$$1=\frac{1}{N^3}\sum_{\mathbf{k},\mathbf{p},\mathbf{p}'}\Lambda_{\mathbf{p}+\mathbf{k}}^2\gamma_{\mathbf{k}-\mathbf{p}'+\mathbf{p}}^{(d)}\gamma_{\mathbf{k}}^{(d)}\frac{Z_{hF}^2}{E_{h\mathbf{k}}}\frac{B_{\mathbf{p}}B_{\mathbf{p}'}}{\omega_{\mathbf{p}}\omega_{\mathbf{p}'}}\left(\frac{F_1^{(1)}(\mathbf{k},\mathbf{p},\mathbf{p}')}{(\omega_{\mathbf{p}'}-\omega_{\mathbf{p}})^2-E_{h\mathbf{k}}^2}-\frac{F_1^{(2)}(\mathbf{k},\mathbf{p},\mathbf{p}')}{(\omega_{\mathbf{p}'}+\omega_{\mathbf{p}})^2-E_{h\mathbf{k}}^2}\right), \tag{4a}$$

$$\frac{1}{Z_{hF}}=1+\frac{1}{N^2}\sum_{\mathbf{p},\mathbf{p}'}\Lambda_{\mathbf{p}+\mathbf{k}_0}^2Z_{hF}\frac{B_{\mathbf{p}}B_{\mathbf{p}'}}{4\omega_{\mathbf{p}}\omega_{\mathbf{p}'}}\left(\frac{F_2^{(1)}(\mathbf{p},\mathbf{p}')}{(\omega_{\mathbf{p}}-\omega_{\mathbf{p}'}-E_{h\mathbf{p}-\mathbf{p}'+\mathbf{k}_0})^2}+\frac{F_2^{(2)}(\mathbf{p},\mathbf{p}')}{(\omega_{\mathbf{p}}-\omega_{\mathbf{p}'}+E_{h\mathbf{p}-\mathbf{p}'+\mathbf{k}_0})^2}+\frac{F_2^{(3)}(\mathbf{p},\mathbf{p}')}{(\omega_{\mathbf{p}}+\omega_{\mathbf{p}'}-E_{h\mathbf{p}-\mathbf{p}'+\mathbf{k}_0})^2}+\frac{F_2^{(4)}(\mathbf{p},\mathbf{p}')}{(\omega_{\mathbf{p}}+\omega_{\mathbf{p}'}+E_{h\mathbf{p}-\mathbf{p}'+\mathbf{k}_0})^2}\right), \tag{4b}$$

respectively, where $\mathbf{k}_0=[\pi,0]$, $\Lambda_{\mathbf{k}}=Zt\gamma_{\mathbf{k}}-Zt'\gamma'_{\mathbf{k}}$, $B_{\mathbf{p}}=2\lambda_1(A_1\gamma_{\mathbf{p}}-A_2)-\lambda_2(2\chi_2^z\gamma'_{\mathbf{p}}-\chi_2)$, $\lambda_1=2ZJ_{\text{eff}}$, $\lambda_2=4Z\phi_2t'$, $A_1=\epsilon\chi_1^z+\chi_1/2$, $A_2=\chi_1^z+\epsilon\chi_1/2$, $\epsilon=1+2t\phi_1/J_{\text{eff}}$, the charge-carrier's particle-hole parameters $\phi_1=\langle h_{i\sigma}^\dagger h_{i+\hat{\eta}\sigma}\rangle$ and $\phi_2=\langle h_{i\sigma}^\dagger h_{i+\hat{\tau}\sigma}\rangle$, the spin-correlation functions $\chi_1^z=\langle S_i^zS_{i+\hat{\eta}}^z\rangle$ and $\chi_2^z=\langle S_i^zS_{i+\hat{\tau}}^z\rangle$,

$$F_1^{(1)}(\mathbf{k},\mathbf{p},\mathbf{p}')=(\omega_{\mathbf{p}'}-\omega_{\mathbf{p}})[n_B(\omega_{\mathbf{p}})-n_B(\omega_{\mathbf{p}'})][1-2n_F(E_{h\mathbf{k}})]+E_{h\mathbf{k}}[n_B(\omega_{\mathbf{p}'})n_B(-\omega_{\mathbf{p}})+n_B(\omega_{\mathbf{p}})n_B(-\omega_{\mathbf{p}'})],$$

$$F_1^{(2)}(\mathbf{k},\mathbf{p},\mathbf{p}')=(\omega_{\mathbf{p}'}+\omega_{\mathbf{p}})[n_B(-\omega_{\mathbf{p}'})-n_B(\omega_{\mathbf{p}})][1-2n_F(E_{h\mathbf{k}})]+E_{h\mathbf{k}}[n_B(\omega_{\mathbf{p}'})n_B(\omega_{\mathbf{p}})+n_B(-\omega_{\mathbf{p}'})n_B(-\omega_{\mathbf{p}})],$$

$$F_2^{(1)}(\mathbf{p},\mathbf{p}')=n_F(E_{h\mathbf{p}-\mathbf{p}'+\mathbf{k}_0})[n_B(\omega_{\mathbf{p}'})-n_B(\omega_{\mathbf{p}})]-n_B(\omega_{\mathbf{p}})n_B(-\omega_{\mathbf{p}'}),$$

$$F_2^{(2)}(\mathbf{p},\mathbf{p}')=n_F(E_{h\mathbf{p}-\mathbf{p}'+\mathbf{k}_0})[n_B(\omega_{\mathbf{p}})-n_B(\omega_{\mathbf{p}'})]-n_B(\omega_{\mathbf{p}'})n_B(-\omega_{\mathbf{p}}),$$

$$F_2^{(3)}(\mathbf{p},\mathbf{p}')=n_F(E_{h\mathbf{p}-\mathbf{p}'+\mathbf{k}_0})[n_B(\omega_{\mathbf{p}'})-n_B(-\omega_{\mathbf{p}})]+n_B(\omega_{\mathbf{p}})n_B(\omega_{\mathbf{p}'}),$$

$$F_2^{(4)}(\mathbf{p},\mathbf{p}')=n_F(E_{h\mathbf{p}-\mathbf{p}'+\mathbf{k}_0})[n_B(-\omega_{\mathbf{p}'})-n_B(\omega_{\mathbf{p}})]+n_B(-\omega_{\mathbf{p}})n_B(-\omega_{\mathbf{p}'}),$$

$n_B(\omega_{\mathbf{p}})$ and $n_F(E_{h\mathbf{k}})$ are the boson and fermion distribution functions, respectively, and the mean-field spin excitation spectrum,

$$\omega_{\mathbf{p}}^2=\lambda_1^2\left[\left(A_4-\alpha\epsilon\chi_1^z\gamma_{\mathbf{p}}-\frac{1}{2Z}\alpha\epsilon\chi_1\right)(1-\epsilon\gamma_{\mathbf{p}})+\frac{1}{2}\epsilon\left(A_3-\frac{1}{2}\alpha\chi_1^z-\alpha\chi_1\gamma_{\mathbf{p}}\right)(\epsilon-\gamma_{\mathbf{p}})\right]+\lambda_2^2\left[\alpha\left(\chi_2^z\gamma'_{\mathbf{p}}-\frac{3}{2Z}\chi_2\right)\gamma'_{\mathbf{p}}+\frac{1}{2}\left(A_5-\frac{1}{2}\alpha\chi_2^z\right)\right]+\lambda_1\lambda_2\left[\alpha\chi_1^z(1-\epsilon\gamma_{\mathbf{p}})\gamma'_{\mathbf{p}}+\frac{1}{2}\alpha(\chi_1\gamma'_{\mathbf{p}}-C_3)(\epsilon-\gamma_{\mathbf{p}})+\alpha\gamma'_{\mathbf{p}}(C_3^z-\epsilon\chi_2^z\gamma_{\mathbf{p}})-\frac{1}{2}\alpha\epsilon(C_3-\chi_2\gamma_{\mathbf{p}})\right], \tag{5}$$

where $A_3=\alpha C_1+(1-\alpha)/(2Z)$, $A_4=\alpha C_1^z+(1-\alpha)/(4Z)$, $A_5=\alpha C_2+(1-\alpha)/(2Z)$, and the spin-correlation functions $C_1=(1/Z^2)\Sigma_{\hat{\eta},\hat{\eta}'}\langle S_{i+\hat{\eta}}^+S_{i+\hat{\eta}'}^-\rangle$, $C_1^z=(1/Z^2)\Sigma_{\hat{\eta},\hat{\eta}'}\langle S_{i+\hat{\eta}}^zS_{i+\hat{\eta}'}^z\rangle$, $C_2=(1/Z^2)\Sigma_{\hat{\tau},\hat{\tau}'}\langle S_{i+\hat{\tau}}^+S_{i+\hat{\tau}'}^-\rangle$, $C_3=(1/Z)\Sigma_{\hat{\tau}}\langle S_{i+\hat{\eta}}^+S_{i+\hat{\tau}}^-\rangle$, and $C_3^z=(1/Z)\Sigma_{\hat{\tau}}\langle S_{i+\hat{\eta}}^zS_{i+\hat{\tau}}^z\rangle$. In order to satisfy the sum rule of the correlation function $\langle S_i^+S_i^-\rangle=1/2$ in the case without the antiferromagnetic long-range order, an important decoupling parameter α has been introduced in the above calculation,[15–17] which can be regarded as the vertex correction. These two Eqs. (4a) and (4b) must be solved simultaneously with other self-consistent equations, then all order parameters, the decoupling parameter α and the chemical potential μ are determined by the self-consistent calculation.[15–17] In this sense, the calculations in this kinetic-energy-driven superconductivity scheme are controllable without using any adjustable parameters. We emphasize that Green's function (3) is obtained within the kinetic-energy-driven superconducting mechanism, although the similar phenomenological expression has been used to discuss the impurity effect in cuprate superconductors.[24,25]

With the charge-carrier BCS formalism [Eq. (3)] under the kinetic-energy-driven superconducting mechanism, we can now introduce the effect of impurity scatterers into the electronic structure. In the presence of impurities, the unperturbed charge-carrier Green's function in Eq. (3) is dressed by impurity scattering,[23]

$$\tilde{g}_I(\mathbf{k},\omega)^{-1}=\tilde{g}(\mathbf{k},\omega)^{-1}-Z_{hF}^{-1}\tilde{\Sigma}(\mathbf{k},\omega), \tag{6}$$

with the self-energy function $\tilde{\Sigma}(\mathbf{k},\omega)=\Sigma_\alpha\Sigma_\alpha(\mathbf{k},\omega)\tau_\alpha$. In this case, the charge-carrier Green's function in Eq. (6) can be explicitly rewritten as,

$$\tilde{g}_I(\mathbf{k},\omega)=\sum_\alpha g_{I\alpha}(\mathbf{k},\omega)\tau_\alpha = Z_{hF}\frac{[\omega-\Sigma_0(\mathbf{k},\omega)]\tau_0+[\bar{\Delta}_{hZ}(\mathbf{k})+\Sigma_1(\mathbf{k},\omega)]\tau_1+[\bar{\xi}_{\mathbf{k}}+\Sigma_3(\mathbf{k},\omega)]\tau_3}{[\omega-\Sigma_0(\mathbf{k},\omega)]^2-[\bar{\xi}_{\mathbf{k}}+\Sigma_3(\mathbf{k},\omega)]^2-[\bar{\Delta}_{hZ}(\mathbf{k})+\Sigma_1(\mathbf{k},\omega)]^2}. \quad (7)$$

Based on this Green's function (7), we[23] have discussed the effect of the extended impurity scatterers on the quasiparticle transport of cuprate superconductors in the superconducting state within the nodal approximation of the quasiparticle excitations and scattering processes, where the main effect on the quasiparticle transport comes from the extended impurity *forward* (or *diagonal*) *scatterers*, and therefore the component of the self-energy function $\Sigma_1(\mathbf{k},\omega)$ has been neglected, while the components of $\Sigma_0(\mathbf{k},\omega)$ and $\Sigma_3(\mathbf{k},\omega)$ have been treated within the framework of the T-matrix approximation. However, it has been demonstrated that the superconducting transition temperature is considerably affected by the out-of-plane impurity scattering in spite of a relatively weak increase in the residual resistivity.[14] This reflects the fact that the superconducting pairing is very sensitive to the out-of-plane impurity scattering, and then the effect of the out-of-plane impurity scattering is always accompanied by breaking of the superconducting pairs. In this case, the out-of-plane impurities can be described as the elastic *off-diagonal scatterers* or *pairing impurity scatterers*. In particular, the modulation of the out-of-plane impurity scattering potential observed in scanning tunneling microscopy experiments[26] has a characteristic wavelength of a few lattice spacings, this may arise because the impurities give rise to an atomic-scale modulation of the charge-carrier *pairing potential* which causes larger, coherence length size fluctuations in the out-of-plane impurity scattering potential.[27] Furthermore, the crude effect of the order parameter modulations on the quasiparticle scattering by allowing the order parameter to be modulated on the four bonds around the impurity has been estimated[25] by adding the off-diagonal scattering potential,

$$\hat{V}=\sum_{\mathbf{k},\mathbf{k}'}[V(\mathbf{k})+V(\mathbf{k}')]\tau_1 = \frac{1}{2}V_0\sum_{\mathbf{k},\mathbf{k}'}[(\cos k_x-\cos k_y)+(\cos k'_x-\cos k'_y)]\tau_1, \quad (8)$$

to the phenomenological d-wave BCS Hamiltonian, then it was shown that the scattering rate is largest at the antinode.

The exact form of the out-of-plane impurity scattering potential is very important for a better understanding of the electronic structure of the out-of-plane impurity-controlled cuprate superconductors. In the following discussions, we determine the form of the out-of-plane impurity scattering potential in terms of the calculation of Dyson's equation. The potential which scatters the electron is taken as summation of impurity potentials $\tilde{V}=\Sigma_l V(\mathbf{r}_i-\mathbf{R}_l)$, where the summation is over all impurity sites l, and then its Fourier transform is obtained[28,29] as $\tilde{V}(\mathbf{q})=\rho_i V(\mathbf{q})\rho(\mathbf{q})$, where

$$\rho(\mathbf{q})=\sum_{\mathbf{k}}h^\dagger_{\mathbf{k}+\mathbf{q}}h_{\mathbf{k}}, \quad (9)$$

$$\rho_i(\mathbf{q})=\sum_l \exp i\mathbf{q}\cdot\mathbf{R}_l, \quad (10)$$

are the charge-carrier density in the Nambu representation and the impurity density, respectively. In the calculation of the self-energy function induced by the impurity scattering, usually it is assumed that the impurities are randomly located and that there is no correlation between their positions.[28,29] In this case, the self-energy function can be obtained as $\tilde{\Sigma}(\mathbf{k},\omega)=\tilde{\Sigma}^{(1)}(\mathbf{k},\omega)+\tilde{\Sigma}^{(2)}(\mathbf{k},\omega)$ within the Born approximation, with the corresponding first-order and second-order self-energy functions are evaluated as,[28,29]

$$\tilde{\Sigma}^{(1)}(\mathbf{k},\omega)=\rho_i\sum_{\mathbf{k}'}\delta_{\mathbf{k}'=0}V(\mathbf{k}')=\rho_i V(0), \quad (11a)$$

$$\tilde{\Sigma}^{(2)}(\mathbf{k},\omega)=\rho_i\sum_{\mathbf{k}',\mathbf{k}''}\delta_{\mathbf{k}'+\mathbf{k}''=0}V(\mathbf{k}')\tilde{g}_I(\mathbf{k}+\mathbf{k}',\omega)V(\mathbf{k}'') = \rho_i\sum_{\mathbf{k}'}V(\mathbf{k}')\tilde{g}_I(\mathbf{k}+\mathbf{k}',\omega)V(-\mathbf{k}'), \quad (11b)$$

where ρ_i is the impurity concentration. As we have mentioned above, the out-of-plane impurities are the off-diagonal scatterers. Although their scattering has a very weak effect on the residual resistivity for cuprate superconductors, a heavy effect on the d-wave superconducting state is observed experimentally.[14] With these considerations, we introduce the following out-of-plane impurity scattering potential:

$$\tilde{V}=\sum_{\mathbf{k}'}V(\mathbf{k}')\tau_1=V_0\sum_{\mathbf{k}'}[\cos k'_x-\cos k'_y]\tau_1. \quad (12)$$

In this case, $V(0)=V_0[\cos(0)-\cos(0)]=0$ [then $\tilde{\Sigma}_1(\mathbf{k},\omega)=0$], and $\tilde{\Sigma}(\mathbf{k},\omega)=\tilde{\Sigma}^{(2)}(\mathbf{k},\omega)$. This form of the out-of-plane impurity scattering potential in Eq. (12) is very similar to that in Eq. (8) used in Ref. 25, and the scattering rate is also largest at the antinode. This is, indeed, confirmed by the quantitative characteristics presented in the following section. With the help of the impurity scattering potential in Eq. (12), the components of the charge-carrier self-energy function $\tilde{\Sigma}(\mathbf{k},\omega)$ are obtained explicitly as,

$$\Sigma_0(\mathbf{k},\omega)=\rho_i\frac{1}{N}\sum_{\mathbf{k}'}|V(\mathbf{k}')|^2 g_{I0}(\mathbf{k}'+\mathbf{k},\omega) = \rho_i\frac{1}{N}\sum_{\mathbf{k}'}|V(\mathbf{k}'-\mathbf{k})|^2 g_{I0}(\mathbf{k}',\omega), \quad (13a)$$

$$\Sigma_3(\mathbf{k},\omega) = -\rho_i \frac{1}{N}\sum_{\mathbf{k}'} |V(\mathbf{k}')|^2 g_{I3}(\mathbf{k}'+\mathbf{k},\omega) = -\rho_i \frac{1}{N}\sum_{\mathbf{k}'+\mathbf{k}} |V(\mathbf{k}'-\mathbf{k})|^2 g_{I3}(\mathbf{k}',\omega), \quad (13b)$$

$$\Sigma_1(\mathbf{k},\omega) = \rho_i \frac{1}{N}\sum_{\mathbf{k}'} |V(\mathbf{k}')|^2 g_{I1}(\mathbf{k}'+\mathbf{k},\omega) = \rho_i \frac{1}{N}\sum_{\mathbf{k}'} |V(\mathbf{k}'-\mathbf{k})|^2 g_{I1}(\mathbf{k}',\omega). \quad (13c)$$

In the charge-spin separation fermion-spin theory,[18] the electron diagonal and off-diagonal Green's functions are the convolutions of the spin Green's function[15–17] $D^{-1}(\mathbf{p},\omega)=(\omega^2-\omega_{\mathbf{p}}^2)/B_{\mathbf{p}}$ and the charge-carrier diagonal and off-diagonal Green's functions in Eq. (7), respectively. These convolutions reflect the charge-spin recombination.[30] Following the previous discussions,[15–17] we can obtain the electron diagonal and off-diagonal Green's functions in the present case. Then the electron spectral function from the electron diagonal Green's function is found explicitly as,

$$A(\mathbf{k},\omega) = \frac{1}{N}\sum_{\mathbf{p}} \frac{B_{\mathbf{p}}}{2\omega_{\mathbf{p}}}\{[n_B(\omega_{\mathbf{p}}) + n_F(\omega_{\mathbf{p}}-\omega)]A_h(\mathbf{p}-\mathbf{k},\omega_{\mathbf{p}}-\omega) - [n_B(-\omega_{\mathbf{p}}) + n_F(-\omega_{\mathbf{p}}-\omega)]A_h(\mathbf{p}-\mathbf{k},-\omega_{\mathbf{p}}-\omega)\}, \quad (14)$$

where A_h is the charge-carrier spectral function, which can be expressed as $A_h = -2\,\mathrm{Im}\, g_I^{dia}(\mathbf{k},\omega)$, with g_I^{dia} obtained from Eq. (7) as,

$$g_I^{dia}(\mathbf{k},\omega) = Z_{hF}\frac{\omega - \Sigma_0(\mathbf{k},\omega) + \bar{\xi}_{\mathbf{k}} + \Sigma_3(\mathbf{k},\omega)}{[\omega-\Sigma_0(\mathbf{k},\omega)]^2 - [\bar{\xi}_{\mathbf{k}} + \Sigma_3(\mathbf{k},\omega)]^2 - [\bar{\Delta}_{hZ}(\mathbf{k}) + \Sigma_1(\mathbf{k},\omega)]^2}. \quad (15)$$

III. ELECTRONIC STRUCTURE OF THE OUT-OF-PLANE IMPURITY-CONTROLLED CUPRATE SUPERCONDUCTORS

Experimentally, it has been shown that the average of the next-nearest-neighbor hopping t' is not appreciably affected by the out-of-plane impurities.[11] In this case, the commonly used parameters in this paper are chosen as $t/J=2.5$ and $t'/t=0.3$. We are now ready to discuss the electronic structure of the out-of-plane impurity-controlled cuprate superconductors and the related superconducting gap. In cuprate superconductors, the information revealed by ARPES experiments[4] has shown that around the nodal $[\pi/2,\pi/2]$ and antinodal $[\pi,0]$ points of the Brillouin zone contains the essentials of the whole low-energy quasiparticle excitation spectrum. In this case, we have performed a calculation for the electron spectral function $A(\mathbf{k},\omega)$ in Eq. (14) at both nodal and antinodal points. The results at (a) the nodal point and (b) the antinodal point with the impurity concentration $\rho_i=0.001$ (solid line), $\rho_i=0.002$ (dashed line), and $\rho_i=0.003$ (dotted line) under the impurity scattering potential with $V_0=50$ J for the charge-carrier doping concentration $\delta=0.15$ are plotted in Fig. 1. For comparison, the corresponding ARPES experimental results[11] for the out-of-plane impurity-controlled cuprate superconductors *Ln*-Bi2201 in the superconducting state are also presented in Fig. 1 (inset). Our results show that the quasiparticle peak is strongly dependent on the impurity concentration, and the peaks at both nodal and antinodal points are suppressed due to the presence of impurity scattering. At the nodal point, there is a sharp superconducting quasiparticle peak near the Fermi energy, however, although the peak at the high impurity concentration is dramatically reduced compared to that at the low impurity concentration, the position of the leading-edge midpoint of the electron spectral function remains almost unchanged. In particular, the position of the leading-edge midpoint of the electron spectral function reaches the Fermi level, indicating that there is no superconducting gap. On the other hand, the spectral intensity from the Fermi energy down to approximately −1.1 J decreases as the impurity concentration increases at the antinodal point, this is the same case as that at the nodal point. However, the position of the leading-edge midpoint of the electron spectral function is shifted toward higher binding energies with increasing impurity concentration, this is in contrast with the behavior observed at the nodal point, and indicates the presence of the superconducting gap. The present results also show that the effect of the out-of-plane impurity scattering is stronger at the antinodal point than at the nodal one, in qualitative agreement with the experimental results.[10,11]

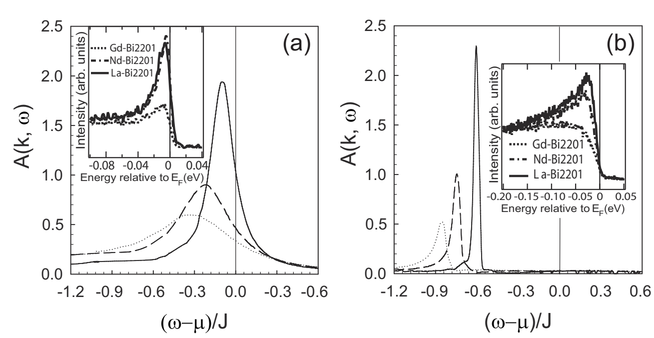

FIG. 1. The electron spectral function at (a) the nodal point and (b) the antinodal point with $\rho_i=0.001$ (solid line), $\rho_i=0.002$ (dashed line), and $\rho_i=0.003$ (dotted line) for $V_0=50$ J at $\delta=0.15$. Inset: the corresponding experimental results taken from Ref. 11.

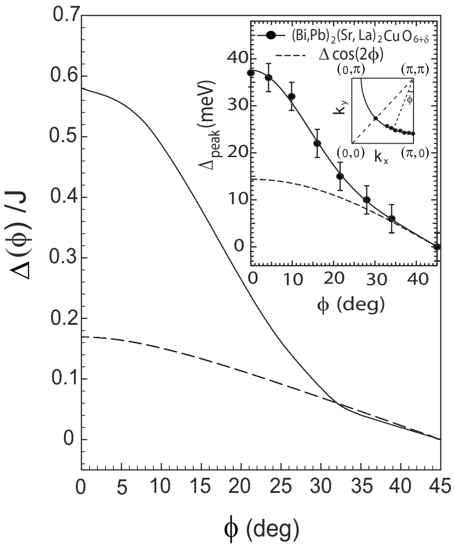

FIG. 2. The superconducting gap as a function of the Fermi surface angle ϕ with $\rho_i=0$ (dashed line) and $\rho_i=0.001$ (solid line) for $V_0=50$ J at $\delta=0.15$. Inset: the corresponding experimental results taken from Ref. 10.

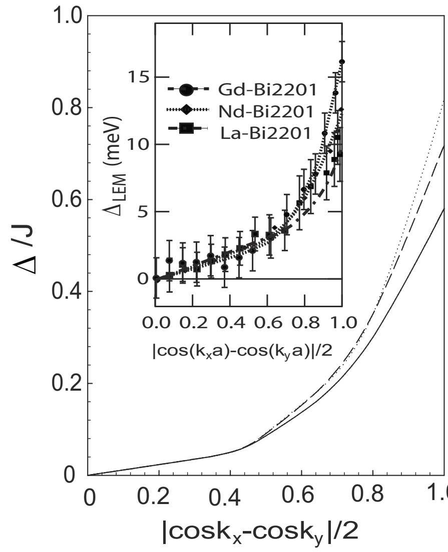

FIG. 3. The superconducting gap as a function of $[\cos k_x - \cos k_y]/2$ with $\rho_i=0001$ (solid line), $\rho_i=0.002$ (dashed line), and $\rho_i=0.003$ (dotted line) for $V_0=50$ J at $\delta=0.15$. Inset: the corresponding experimental results taken from Ref. 11.

The behavior of the electron spectrum in Fig. 1 indicates an enhancement of the superconducting gap in the antinodal region by the impurity scattering. To show this point clearly, we have calculated the electron spectral function $A(\mathbf{k},\omega)$ along the direction $[\pi,0]\rightarrow[\pi/2,\pi/2]$, and then employed the shift of the leading-edge midpoint as a measure of the magnitude of the superconducting gap at each momentum just as it has been done in the experiments.[10,11] The results for the extracted superconducting gap as a function of the Fermi surface angle ϕ, defined in the inset, with the impurity concentration $\rho_i=0$ (dashed line) and $\rho_i=0.001$ (solid line) under the impurity scattering potential with $V_0=50$ J for the charge-carrier doping concentration $\delta=0.15$ are plotted in Fig. 2 in comparison with the corresponding ARPES experimental results for the out-of-plane impurity-controlled cuprate superconductor $(Bi,Pb)_2(Sr,La)_2CuO_{6+\delta}$ in the superconducting state[10] (inset). It is clearly shown that the superconducting gap Δ increases with the Fermi surface angle decreasing from 45° (node) to 0° (antinode). Although the superconducting gap in the presence of the impurity scattering is basically consistent with the d-wave symmetry, it is obvious that there is a strong deviation from the monotonic d-wave form around the antinodal region. In particular, this strong deviation is mainly caused by a remarkable enhancement of the superconducting-gap value around the antinodal region, in qualitative agreement with the experimental results.[10,11] In other words, the superconducting gap around the antinodal region is strongly enhanced by the impurity scattering, whereas around the nodal region its value remains the same. As a consequence, the well-pronounced deviation from the monotonic d-wave superconducting-gap form in the out-of-plane impurity-controlled cuprate superconductors is mainly caused by the effect of the out-of-plane impurity scattering. This is also the reason why the superconducting-gap function for very high quality samples of the cuprate superconductor $La_{1-x}Sr_xCuO_4$ has a monotonic d-wave form.[31]

For a better understanding of the impurity-concentration dependence of the deviation from the monotonic d-wave superconducting-gap function, we have made a series of calculations for the superconducting gap at different impurity concentration levels, and the results of the superconducting gap as a function of the monotonic d-wave function $[\cos k_x - \cos k_y]/2$ with the impurity concentration $\rho_i=0001$ (solid line), $\rho_i=0.002$ (dashed line), and $\rho_i=0.003$ (dotted line) under the impurity scattering potential with $V_0=50$ J for the charge-carrier doping concentration $\delta=0.15$ are plotted in Fig. 3 in comparison with the corresponding ARPES experimental results for the out-of-plane impurity-controlled cuprate superconductors Ln-Bi2201[11] (inset). Obviously, our results show that the magnitude of the deviation from the monotonic d-wave superconducting-gap form around the antinodal region increases with increasing impurity concentration, in qualitative agreement with the experimental results.[10,11] This strong out-of-plane impurity effect in the antinodal region is also consistent with scanning tunneling spectroscopy results,[32] where the average of the superconducting-gap size, which corresponds to the antinodal superconducting gap in the ARPES spectra, increases with increasing impurity concentration.

Within the framework of the kinetic-energy-driven superconducting mechanism[17] in the presence of the out-of-plane impurities, our present results show that the out-of-plane impurity scattering potential (12), in which the impurities modulate the pair interaction locally, gives qualitative agreement with respect to the main features observed in the ARPES measurements on the out-of-plane impurity-controlled cuprate superconductors in the superconducting state. Although this out-of-plane impurity effect in cuprate superconductors can also be discussed starting directly from a phenomenological d-wave BCS formalism,[25,27] in this paper we are primarily interested in exploring the general notion of the effects of the out-of-plane impurity scatterers in the kinetic-energy-driven cuprate superconductors in the superconducting state. The qualitative agreement between the present theoretical results and ARPES experimental data also indicates that the presence of the out-of-plane impurities has a crucial impact on the electronic structure of cuprate superconductors. On the other hand, we emphasize that the quasiparticle scattering rate in the antinodal region is strongly increased by the impurity scattering potential (12), while the nodal quasiparticles are very weakly scattered by the impurity scattering potential (12), this is why the superconducting transition temperature is considerably affected by the out-of-plane impurity scattering in spite of a relatively weak increase in the residual resistivity,[14] since the transport properties are mainly governed by the quasiparticles in the nodal region.

IV. SUMMARY

In conclusion, we have shown very clearly in this paper that if the out-of-plane impurity scattering is taken into account within the framework of the kinetic-energy-driven d-wave superconductivity,[17] the quasiparticle spectrum of the t-J model calculated based on the off-diagonal impurity scattering potential (12) *per se* can correctly reproduce some main features found in the ARPES measurements on the out-of-plane impurity-controlled cuprate superconductors in the superconducting state.[10,11] In the presence of the out-of-plane impurities, although both sharp superconducting coherence peaks around the nodal and antinodal regions are suppressed, the effect of the impurity scattering is stronger in the antinodal region than that in the nodal region, this leads to a strong deviation from the monotonic d-wave superconducting-gap form in the out-of-plane impurity-controlled cuprate superconductors.

Finally, we have noted that within a phenomenological BCS approach, the electron spectral properties of the underdoped cuprates as resulting from a momentum-dependent pseudogap in the *normal state* have been discussed,[6] where a normal-state pseudogap function deviating from the monotonic d-wave pseudogap form has been used to fit the ARPES experimental data in the normal state. It has been shown[13,33] that there are some subtle differences for different families of underdoped cuprates in the normal state, and therefore it is possible that the pseudogap in the normal state is effected by the impurity scattering as well.

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