Coexistence of superconductivity and antiferromagnetism in self-doped bilayer \( t-t' \)-\( J \) model

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I. INTRODUCTION

High-\( T_c \) superconductors (HTSC) have one or more CuO\(_2\) planes in a conducting block, which is separated by charge-reservoir blocks. In HTSC with more than three CuO\(_2\) planes in a unit cell, there exist two inequivalent types of CuO\(_2\) planes: pyramidally-coordinated-outter planes (OP) and square-coordinated-inner planes (IP). The nuclear magnetic resonance (NMR) studies found that the hole density in OP is larger than that in IP.\(^8\) An example of these is the five-layered HgBa\(_2\)Ca\(_4\)Cu\(_8\)O\(_{y}\)\(_3\), in which the optimally doped OPs are superconducting (SC) with \( T_c = 108K \), while the three IPs have an antiferromagnetic (AFM) moment.\(^{8,9}\) Although the SC planes are separated by the AFM ones, the Josephson coupling through the AFM planes stabilizes the superconductivity as a bulk.\(^2\)

Another kind of multilayered HTSC is the four-layered Ba\(_2\)Ca\(_4\)Cu\(_3\)O\(_{8}\)(O\(_{y}\)F\(_{1-x}\))\(_2\) (F0234)\(^{8,9}\). Especially for \( x = 0 \), a nominal Cu valence is +2 on the canonical chemical formula. Thus, this material is expected to be a Mott insulator, although the superconductivity with \( T_c = 60K \) takes place.\(^{8,9}\) This compound, F0234, has four CuO\(_2\) planes, among which two OP’s have apical F atoms, while the two IP’s do not. Angle-resolved-photoemission-spectroscopy (ARPES) experiments observed two Fermi surfaces (FS’s), whose volumes in the first Brillouin zone correspond to electron- and hole-doped FS’s.\(^{8,9}\) This would be the first self-doped high \( T_c \) superconductor with an electron- and a hole-doped CuO\(_2\) planes in the same crystal. It is also found that the superconducting (SC) gap on the electron-doped FS is twice as large as that on the hole-doped one.\(^{10}\)

On the other hand, it is known that doped holes make a FS around the nodal region,\(^{12,13,14,15}\) while doped electrons create pockets around the anti-nodal region.\(^{10}\) Theoretical studies by the variational Monte Carlo method\(^{10}\) and the exact diagonalization method\(^{10,12}\) elucidate that the asymmetry between hole- and electron-doped cuprates results from second neighbor hopping \((t')\) and third neighbor one \((t'')\) in the CuO\(_2\) plane. Here, the question arises: what is the ground state of the self-doped bilayer cuprates, where one plane is electron-doped and the other is hole-doped, and how are the FS’s and their asymmetry?\(^{10}\)

To answer these questions, the self-doped \( t-t' \)-\( J \) model is examined by the slave-boson mean-field theory. The two different types of planes are connected by an inter-layer hopping renormalized by electron-electron correlation. A site potential making the charge imbalance between two planes is included. Note that the hopping of a single spin between a holon- and a doublon-sites picks up extra minus sign as compared to that between a holon- and a single-occupied site.\(^{13}\) This doublon effect leads to a spin singlet states between the two planes.

In an undoped bilayer system, both planes have same amount of carriers due to the self-doping, although one type of carrier is hole and the other is electron. Our results show that in both electron- and hole-doped planes, AFM and SC coexist. Other authors studied the undoped case with no interlayer hopping.\(^{21,22}\) We examine the doped case with holes as well. In the doped case, the numbers of carriers in each plane becomes imbalanced, i.e. doublon density decreases and holon density increases with hole doping. As a result, the magnitudes of order parameters become more dissimilar compared to the undoped case. Two FS’s in the self-doped bilayer look like a composite of hole- and electron-doped cuprates. However, we cannot find the FS splitting in the nodal direction, since one band becomes very flat due to the AFM orders.

This paper is organized as follows. In Sec. II we introduce the bilayer \( t-t' - J \) model with an interlayer hopping and a site potential, and present the slave-boson mean-field scheme. In Sec. III, we discuss self-consistent mean-field solutions for both undoped and doped cases of self-doped bilayer system. Coexistent phase of SC and AFM orders are discussed from the viewpoint of doping and charge imbalance. FS and dispersion relation of
spinons are shown in the AFM ordered phase. In Sec. we will give summary and discussion.

II. MODEL AND METHOD

The model we apply to study the self-doped bilayer system is written as:

\[
H = H_\parallel + H_W + H_\perp,
\]

where \(c^{(l)}_{i\sigma}\) is the electron annihilation (creation) operator with spin \(\sigma\) at site \(i\) in the \(l\)-th plane. The electron number in each plane is denoted by \(n^{(l)}_i = \sum_\sigma c^{(l)*}_{i\sigma} c^{(l)}_{i\sigma}\), and the averaged electron density is defined as, \(n = (n^{(1)} + n^{(2)}/2\). The signs, \((ij)\) and \((ij)\), run over nearest- and next-nearest neighbor sites, respectively. The chemical potential \(\mu\) and the site potential \(W\) control the charge imbalance. Below, we take \(J/t = 1/3\) and \(t'/t = -0.4\).

The interlayer hopping in Eq. (1) has the dispersion relation in the momentum space, \(\varepsilon_{\perp, k} = (t_\perp/4) (\cos k_x - \cos k_y)^2\), where \(t_\perp\) is the amplitude without renormalization.\[2,11,13,15,21,22,23\]

We treat Hamiltonian (1) in the slave-boson mean-field theory. The electron operator is represented as, \(c^{(l)}_{i\sigma} = f^{(l)}_{i\sigma} h^{(l)}_i + \sigma f^{(l)}_{i\sigma} d^{(l)}_{i\sigma}\), with \(h^{(l)}_i\) and \(d^{(l)}_{i\sigma}\) being the bosonic holon and doublon operators, respectively.\[22,24\]

The fermionic spinon operator is denoted by \(f^{(l)}_{i\sigma}\). In the self-doped case, we assume that one plane is hole-doped and the other is electron-doped. For the hole-doped plane, as there is no bond, the electron operator can be expressed as, \(c^{(l)}_{i\sigma} = f^{(l)}_{i\sigma} h^{(l)}_i\), with the constraint, \(h^{(l)}_i h^{(l)*}_i + \sum_\sigma f^{(l)*}_{i\sigma} f^{(l)}_{i\sigma} = 1\), while for the electron-doped plane, as there is no holon, the electron operator can be expressed as, \(c^{(l)}_{i\sigma} = \sigma f^{(l)}_{i\sigma} d^{(l)}_{i\sigma}\), with the constraint, \(d^{(l)}_i d^{(l)*}_i + \sum_\sigma f^{(l)*}_{i\sigma} f^{(l)}_{i\sigma} = 1\). Since we are interested in the electronic states at low temperatures, the boson condensation is assumed in each plane, i.e., \(\langle h^{(l)}_i \rangle = \langle f^{(l)}_{i\uparrow} \rangle = \sqrt{\delta^{(l)}_{h}}\) and \(\langle d^{(l)}_i \rangle = \langle d^{(l)}_{i\downarrow} \rangle = \sqrt{\delta^{(l)}_{d}}\), where \(\delta^{(l)}_h\) and \(\delta^{(l)}_d\) are the holon and doublon densities.

To decouple the Hamiltonian, we introduce the order parameters in the electron- and the hole-doped planes as, \(\Delta^{(l)}_h = \langle f^{(l)}_{i\uparrow} f^{(l)}_{i\downarrow} \rangle - \langle f^{(l)}_{i\uparrow} \rangle \langle f^{(l)}_{i\downarrow} \rangle\), \(\chi^{(l)}_h = \langle c^{(l)}_{i\sigma} c^{(l)*}_{i\sigma} \rangle\), \(m^{(l)} = (-1)^{l+1}(n^{(l)}_{i\uparrow} - n^{(l)}_{i\downarrow})\), where \(\eta = x, y\) indicates the nearest-neighbor sites. Although the magnetic order in real materials may be quite complicated, we only consider the commensurate antiferromagnetic orders for simplicity. As the interlayer hopping may induce a weak AFM correlation between the two planes, the staggered AFM order has a sign difference between the two planes in our definition. All parameters are assumed to be real and the SC pairing symmetry is \(d\)-wave.

The Hamiltonian (1) based on the above treatment is decoupled in the momentum space as follows:

\[
H_{MF} = \sum_{l,k,\sigma} \varepsilon^{(l)}_k f^{(l)}_{i\sigma} f^{(l)}_{k\sigma} + \varepsilon^{(l)}_k f^{(l)}_{i\sigma} f^{(l)}_{k\sigma} + h.c.\]

\[
-\frac{J}{2} \sum_{l,k} \Delta^{(l)}_k \eta_k (f^{(l)}_{i\uparrow} f^{(l)}_{k\downarrow} - f^{(l)}_{i\downarrow} f^{(l)}_{k\uparrow} + h.c.)\]

\[
-\sum_{k,\sigma} \sqrt{\delta^{(l)}_{h}} \delta^{(l)}_{d} \varepsilon_{\perp, k} \cdot \sigma\]

\[
\times \left(f^{(l)}_{\sigma} f^{(l)}_{k\sigma} + f^{(l)}_{\sigma} f^{(l)}_{k\sigma} + h.c.\right),\]

\[
+ JN \sum_{l} \left(\Delta^{(l)2} + \frac{1}{2} \chi^{(l)2} + \frac{1}{2} m^{(l)2} + \frac{1}{2} n^{(l)2} \right),\]

where \(\gamma_k = 2(\cos k_x + \cos k_y), \zeta_k = 4 \cos k_x \cos k_y, \zeta_k = 4 \cos k_x \cos k_y, \) and \(k\) runs over the magnetic Brillouin zone with \(|k_x \pm k_y| \leq \pi\). \(Q = (\pi, \pi)\) is the magnetic vector and \(N\) is the total number of lattice sites. \(\delta^{(l)}_h\) is the renormalization factor of \(t^{(l)}_\perp\). Here, we assumed the \(l=1\) (2) is the hole (electron) doped plane.

We note that as seen in the fourth term in Eq. (5), the interlayer hopping in self-doped bilayer system may induce an interlayer singlet-paring, which can be defined as, \(\Delta_p = \langle f^{(l)}_{\uparrow} f^{(l)}_{\downarrow} - f^{(l)}_{\downarrow} f^{(l)}_{\uparrow} \rangle\). The momentum dependence of dispersions is given by \(\varepsilon^{(l)}_k = -(t^{(l)}_h + \frac{1}{2} J \chi^{(l)}_{\downarrow} \gamma_k - t^{(l)}_d \chi^{(l)}_h (\mu + J n^{(l)}_h - W), \varepsilon^{(l)}_k = \langle f^{(l)}_{\sigma} f^{(l)}_{k\sigma} + f^{(l)}_{\sigma} f^{(l)}_{k\sigma} + h.c.\rangle,\) where \(n^{(l)}_h = \sum_\sigma f^{(l)}_{\sigma} f^{(l)}_{\sigma}\) and \(n^{(l)}_d = \sum_\sigma f^{(l)}_{\sigma} f^{(l)}_{\sigma}\) are spinon densities in plane 1 and 2, respectively. For the given total electron number \(n\) and site potential \(W\), the mean-field parameters \(\Delta^{(l)}_h, \chi^{(l)}_h\), and \(m^{(l)}\), the charge density in each plane \(\delta^{(l)}_h, \delta^{(l)}_d\) and the chemical potential \(\mu\) are self-consistently determined in numerical calculations.

III. RESULTS AND DISCUSSION

A. Self-doped bilayer at half-filling (n=1)

First, we focus our study on the undoped case, i.e., \(n = 1\). In this case, the holon density in hole-doped plane is equal to the doublon density in electron-doped plane, i.e., \(\delta^{(l)}_h = \delta^{(l)}_d\). Figure 1 shows the results of the
d-wave pairing amplitude \((\Delta^{(l)})\), the uniform bond order parameter \((\chi^{(l)})\), the AFM order parameter \((m^{(l)})\), the site potential \((W)\) and the interlayer singlet pairing amplitude \((\Delta_p)\) as functions of the holon (doublon) density \(\delta^{(1)}_h \text{ (} \delta^{(2)}_d \text{)}\) for various values of the interlayer hopping parameter \((t_\perp)\), \(\Delta^{(l)}\), \(\chi^{(l)}\), and \(m^{(l)}\) depend very weakly on \(t_\perp\), particularly for small \(W\) (small \(\delta^{(1)}_h \text{ and} \ \delta^{(2)}_d\)). \(\Delta_p\) increases with \(t_\perp\). When \(t_\perp = 0\), \(\Delta_p = 0\). Fig. 4 (a) shows the relation between \(W\) and \(\delta^{(1)}_h \text{ (} \delta^{(2)}_d\text{)}\). When \(W = 0\), there is no charge imbalance between the two planes, i.e., \(\delta^{(1)}_h = \delta^{(2)}_d = 0\). In this case, both planes are at half-filling, with \(m^{(l)} = 1\) and \(\Delta^{(l)} = \chi^{(l)} = 0\). The ground state is an AFM insulator. When \(\delta^{(1)}_h = \delta^{(2)}_d = 0\), \(\Delta_p\) becomes zero, that is, the planes are decoupled regardless of the interlayer hopping and the planes are coupled only for finite \(\delta^{(1)}_h \text{ (} \delta^{(2)}_d\text{)}\). When \(W\) increases, the charge densities \(\delta^{(1)}_h \text{ and} \ \delta^{(2)}_d\) increase from zero. The staggered AFM magnetization decreases with \(\delta^{(1)}_h \text{ (} \delta^{(2)}_d\text{)}\), while the d-wave paring amplitude \((\Delta^{(l)})\) and the uniform bond order parameter \((\chi^{(l)})\) both increase. \(m^{(1)}\) and \(m^{(2)}\) are almost the same in the region \(0 < \delta^{(1)}_h \text{ (} \delta^{(2)}_d\text{)} \lesssim 0.15\), and then \(m^{(1)}\) decreases faster than \(m^{(2)}\) and vanish at around \(\delta^{(1)}_h = \delta^{(2)}_d \sim 0.2\). It is seen that for \(0 < \delta^{(1)}_h \text{ (} \delta^{(2)}_d\text{)} \lesssim 0.2\), both electron- and hole-doped planes are the coexistent state of AFM and SC. When AFM order vanishes, both planes are superconducting.

Here, we mention yet another solution, where \(\delta^{(1)}_h = \delta^{(2)}_d \neq 0\) even for \(W = 0\), and \(m^{(2)} \gg m^{(1)} \sim 0\). This may be a possible phase separation, where electrons are spontaneously transferred from the hole-doped plane to the electron-doped one to gain an energy of magnetic exchange interaction without the site potential. Since this solution is found in a limited (unphysical) parameter region, we do not discuss below.

**B. Hole-doped case \((n < 1)\)**

Next we investigate the doped case in the self-doped bilayer system. In the doped case, i.e., \(n \neq 1\), the holon density \(\delta^{(1)}_h\) is not necessarily equal to doublon density \(\delta^{(2)}_d\). Figure 2 shows the results of \(\delta^{(1)}_h \text{, } \Delta^{(l)}, \chi^{(l)}, \text{ and } m^{(l)}\) as functions of the total electron density \(n\) for a given \(W/t = 0.05\). From Fig. 2 (a), we see that for small doping of holes, \(0.97 \leq n < 1\), both \(\delta^{(1)}_h\) and \(\delta^{(2)}_d\) increase. This means that holes first go into hole-doped plane, while some electrons are transferred from hole-doped plane to electron-doped plane. The kinetic energy gains in this case. Upon further doping of holes into the system, holes go into both planes, and \(\delta^{(1)}_h\) increases while \(\delta^{(2)}_d\) decreases. Due to the change of charge density, the staggered AFM magnetization in hole-doped plane \((m^{(1)})\) decreases while \(m^{(2)}\) increases. For \(0.86 \lesssim n < 1\), both electron- and hole-doped planes are the coexistent state of AFM and SC. For \(0.86 \lesssim n \lesssim 0.97\), the AFM order in hole-doped plane is small, and \(m^{(1)}\) decreases fast with \(t_\perp\). When \(t_\perp = 0\), \(m^{(1)}\) becomes zero in this region. At a critical point \(n \sim 0.86\), doublon vanishes \((\delta^{(2)}_d = 0)\), and electron-doped plane goes into AFM insulator phase; simultaneously \(m^{(1)}\) becomes zero, and hole-doped plane goes into the superconducting phase. Above the critical point \((n < 0.86)\), both planes are hole-doped.

So far we have presented results for both undoped and doped cases. Now we discuss the phase diagram. Fig. 3 shows the phase diagram in the \(W-n\) plane for \(t_\perp/t = 0.5\). The phase diagram is divided into three parts. For small doping \((n \sim 1)\) and large site potential \(W\), the charge imbalance is large and both planes are SC; for small \(W\) and small \(n\), both planes are hole-doped; for intermediate \(W\) and \(n\), both electron- and hole-doped planes are the coexistent state of AFM and SC. In the undoped case \((n = 1)\), with increasing \(W\), \(\delta^{(1)}_h = \delta^{(2)}_d\) increases and there is a transition from coexistent state of AFM and SC to SC in both planes. In the doped case
with $n = 0.85$, both planes are hole-doped for small $W$. When $W$ increases above a critical value of $W_C$, electrons move from hole-doped plane to electron-doped plane and both planes are the AFM and SC coexistent state due to self-doping.

C. Spinon Fermi surfaces and dispersion relation

As for the asymmetry between the hole- and the electron-doped cuprates, one of distinguished observations is the FS pocket, which is located around the nodal region in hole-doped cuprates$^{12,13,14,15}$ and the anti-nodal region in electron-doped ones$^{16}$. It is found that this asymmetry originates from the different signs of $t'$ and $t^n$.$^{17,18,19,20}$ On the other hand, the multilayered cuprates doped with holes show the interlayer splittings of FS$^{23,24,25,26,27,30,31,32}$. In the nodal direction, the splitting means the charge imbalance between IP and OP, while those around the anti-nodal regions are ascribed to a magnitude of interlayer hopping renormalized by the charge imbalance$^{29}$. Interesting is that the two asymmetric planes are combined by the interlayer hopping in the self-doped bilayer system.

In Fig. 2 the spinon FS's and dispersion relations of self-doped bilayer systems are plotted for some doping rates in the AFM phase. Details of parameters are included in the caption of Fig. 2. Near the half-filling given by, $n=0.98$, $\delta_{h}^{(1)}=0.130$, and $\delta_{d}^{(2)}=0.090$, two FS pockets appear in the nodal and the antinodal regions shown in Fig. 2(a). It looks like a composite of hole- and electron-doped cuprates. As shown in Fig. 2(c) and (d), the AFM moment in the hole-doped plane markedly becomes small, $m^{(1)}=0.47$ and $m^{(2)}=0.68$. With increasing hole density in the bilayer as $n=0.95$ and 0.9, the hole-doped like FS becomes larger as shown in Fig. 2(b) and (c), and the AFM moment in the hole-doped plane markedly becomes small, $m^{(1)}=0.05$ and 0.01. As a result, the separation of four bands close on each another as shown in Figs. 2(f) and (g). On the other hand, since the AFM moment in the electron-doped plane still large, $m^{(2)}=0.73$ and 0.95, two among four bands become quite flat. Finally, for $n=0.85$, both plane becomes hole-doped. Interesting is that we cannot find the interlayer splitting in the nodal direction as shown in Fig. 2(d), although it is found in the normal metallic phase$^{30,31}$. The missing of FS splitting is caused by the AFM moment in the 2nd plane, which make a band flat as shown in Fig. 2(h).
and SC order parameters are imposed to be zero. In (d) and (f) $\delta$ing the slave-boson mean-field theory. Each plane is de-

FIG. 4: FS’s and dispersion relations of self-doped bi-

layer system; (a) and (e) $n=0.98$, $\delta_{1}^{(1)}=0.130$, $\delta_{2}^{(1)}=0.090$; (b) and (f) $n=0.95$, $\delta_{b}^{(1)}=0.180$, $\delta_{d}^{(2)}=0.080$; (c) and (g) $n=0.90$, $\delta_{b}^{(1)}=0.225$, $\delta_{d}^{(2)}=0.025$; (d) and (h) $n=0.85$, $\delta_{b}^{(1)}=0.25$, $\delta_{d}^{(2)}=0.05$. In these figures, $W/t=0.05$ and $t_{\perp}/t=0.5$ are fixed, and SC order parameters are imposed to be zero. In (d) and (h), both two planes are in hole-doped regions.

IV. SUMMARY AND DISCUSSION

We have studied the bilayer self-doped cuprates by us-

scribed by the $t$-$t'$-$J$ model, and the interlayer hopping and a site potential are included. In an undoped bilayer system, both planes have same amount of carriers due to the self-doping, although one type of carrier is hole and the other is electron. Our results show that in both electron- and hole-doped planes, AFM and SC coexist. In the doped cases with holes, the numbers of carriers in each plane becomes imbalanced, i.e. doublon density decreases and holon density increases with hole doping. The magnitudes of order parameters become more dis-
similar compared to the undoped case. At some critical doping of holes, the doublon disappears and the electron layer becomes an insulator. This effect might be useful for a p-n junction made of the electron- and hole-doped layers if we could control the doping near this value. Two FS’s in the self-doped bilayer look like a composite of hole- and electron-doped cuprates. However, we cannot find the FS splitting in the nodal direction even in the bilayer system, since one band becomes very flat due to the AFM orders.

In the ARPES experiment on F0234, two FS’s sur-

rounding the $(\pi, \pi)$ point and the FS’s splitting in the nodal direction are observed. The doping rate in each plane may be optimal or overdoped. In such a case, the FS should enclose the $(\pi, \pi)$ point like as Bi-compounds, not like as a pocket. On the other hand, the NMR study observed the magnetic moment, which could not exist around the optimum doping region. Although our model is a bilayered system, it involves essential points of multilayered cuprates. In addition to the bilayered system, the four-layered $t$-$t'$-$J$ model was examined to find the FS splitting in the nodal region. However, we could not find it in the self-doped four-layered system, while it was found in the four hole-doped layers. The contradiction between experiment and theory remains to be resolved in the future.

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