

Coexistence of magnetism and superconductivity in a t - J bilayer

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We investigate coexistence of antiferromagnetic and superconducting correlations in bilayered materials using a two-dimensional t - J model with couplings across the layers using variational Monte Carlo calculations. It is found that the underdoped regime supports a coexisting phase, beyond which the (d -wave) superconducting state becomes stable. Further, the effects of interplanar coupling parameters on the magnetic and superconducting correlations as a function of hole doping are studied in detail. The magnetic correlations are found to diminish with increasing interplanar hopping away from half filling, while the exchange across the layers strengthens interplanar antiferromagnetic correlations both at and away from half filling. The superconducting correlations show more interesting features where larger interplanar hopping considerably reduces planar correlations at optimal doping, while an opposite behavior, i.e., stabilization of the superconducting state, is realized in the overdoped regime, with the interplanar exchange all the while playing a dormant role.

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I. INTRODUCTION

The mechanism leading to electron pairing in copper oxide superconductors has stimulated a great deal of speculation. The manifestation of planar antiferromagnetism in the CuO_2 layers has provided motivation to study the role and importance of antiferromagnetic (AF) interactions between Cu^{2+} spins and their intimate relevance to superconductivity.¹ Doping with holes in these insulating cuprates results in destruction of long range order; however, short range antiferromagnetic correlations between the copper moments survive. Further doping leads to the emergence of a superconducting (SC) state.

Thus, the interplay of AF and SC phases has generated much attention. A phenomenological $\text{SO}(5)$ theory has attempted to unify antiferromagnetism and superconductivity owing to their proximity in the phase diagram.^{2,3} The basic assumption of the theory is that these two phases share a common microscopic origin and hence both demand treatment at an equal footing. A number of experimentally observed features, such as the vortex state, a resonant peak in SC state from neutron scattering data for optimally and underdoped samples, etc., have provided ample credence to the theory. However, a microscopic theory in this regard is still lacking.

A natural extrapolation of finding the connection between AF and SC is the issue of their coexistence which seems more crucial and calls for attention. A large volume of work exists that focuses on the various details of the coexistence phenomenon. Some of the theoretical attempts include mean field studies of t - J and Hubbard-like models which confirm the coexistence of magnetic and superconducting order.^{4,5} The coexistence is suggestive of the presence of short range AF correlations in SC state that are probed by inelastic neutron scattering experiments via an enhanced scattering intensity near the AF wave vector (π, π) .⁶⁻⁹

The coexistence issue has been revived recently in the context of bilayer (and multilayer) cuprates.^{5,8} While acknowledging the planar correlations perhaps dominate the physical properties of these superconductors, the role of in-

terlayer couplings and their relevance to the coexistence phenomena for layered materials have been heavily emphasized. Intimately connected to this is the question of whether the superconducting correlations originate from AF spin fluctuations¹⁰⁻¹² or via a electron-phonon mediated pairing enhanced by interlayer tunneling.¹³ However, both these mechanisms cannot be operative together.

The next fundamental question is the symmetry of the superconducting gap function. Even with sufficient experimental evidence for a $d_{x^2-y^2}$ pairing for a planar materials (for a comprehensive review on the subject, see Ref. 14), for bilayers, the pairing symmetry is still unclear. Several variational calculations¹⁵⁻¹⁷ performed over the years have provided nourishment to a $d_{x^2-y^2}$ -wave pairing scenario, and a reasonably broad window of carrier concentration has been identified in planar systems where magnetic and SC orders coexist. Similar studies in the context of bilayers are lacking, which provides motivation for us to investigate a bilayer t - J model via variational Monte Carlo (VMC) technique.

Our goal in this work is to examine the coexistence of antiferromagnetism and superconductivity in t - J bilayers using VMC and to study the magnetic and superconducting correlations in the variational ground state. We further intend to investigate the dependence of these properties on interlayer coupling strengths. In a recent paper,²³ to determine the most suitable pairing symmetry of the SC state in t - J bilayers, we investigated the stability of various pairing symmetries, e.g., (a) $\Delta(\cos k_x - \cos k_y)$ (d wave), (b) $\Delta_{\parallel}(\cos k_x - \cos k_y) + \Delta_{\perp} \cos k_z$, and (c) $\Delta_{\parallel}(\cos k_x - \cos k_y) + \Delta_{\perp}(1 - \cos k_z)$. Another function discussed in connection with bilayer materials but not included in our previous study is the s^{\pm} state [$\Delta_k = \pm \Delta(\cos k_x + \cos k_y)$ with “+” sign for $k_z=0$ and “-” for $k_z=\pi$], which has s -wave symmetry and opposite signs in the bonding ($k_z=0$) and antibonding bands ($k_z=\pi$).^{18,19} This state possesses the merit of explaining the resonance peak at 41 meV obtained in neutron scattering experiments.^{6,20-22} In this paper, we consider also this pairing symmetry in the search for most stable ground state in bilayers.

Here, we state the main results obtained by us. The long range AF order coexists with superconductivity in the under-

doped regime. In the coexisting phase, not only the AF but SC correlations are also significantly stronger as compared to that in the pure SC (d -wave) state. Larger interlayer hopping frequency reduces planar SC correlations in the optimally doped phase, whereas it enhances it in the overdoped regime, while the effect of interlayer exchange on SC correlations is minimal for the range of the parameter values considered in our paper.

Our paper is organized as follows. Section II introduces the t - J model for bilayers and discusses the most suitable variational wave function to be used for our calculations. A brief note on the numerics used and an elaborate discussion on the results appear in Sec. III. The effects of interplanar coupling parameters have been emphasized in magnetic, superconducting, and coexisting phases. Section IV concludes with a brief summary of the results obtained in this paper.

II. HAMILTONIAN AND THE VARIATIONAL WAVE FUNCTION

The t - J Hamiltonian for a bilayer can be written as

$$\begin{aligned} \mathcal{H} = & -t \sum_{\langle i,j \rangle \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + \text{H.c.}) + J \sum_{\langle i,j \rangle} \left(\mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4} n_i n_j \right) \\ & - t_\perp \sum_{\langle\langle i,k \rangle\rangle \sigma} (c_{i\sigma}^\dagger c_{k\sigma} + \text{H.c.}) + J_\perp \sum_{\langle\langle i,k \rangle\rangle} \left(\mathbf{S}_i \cdot \mathbf{S}_k - \frac{1}{4} n_i n_k \right), \end{aligned} \quad (1)$$

where t and J are the planar hopping and exchange integrals, respectively, while t_\perp and J_\perp are the corresponding interplanar parameters. $c_{i\sigma}$ ($c_{i\sigma}^\dagger$) annihilates (creates) an electron of spin σ at site i , $n_i = \sum_\sigma c_{i\sigma}^\dagger c_{i\sigma}$, and \mathbf{S}_i is the spin operator at site i given by $S_i^\alpha = \psi_i^\dagger (\frac{1}{2} \boldsymbol{\sigma}_\alpha) \psi_i$, $\psi_i^\dagger = (c_{i\uparrow}^\dagger \ c_{i\downarrow}^\dagger)$ and $\boldsymbol{\sigma}_\alpha$ (with $\alpha = x, y, z$) are the Pauli spin matrices. The summation indices $\langle i, j \rangle$ and $\langle\langle i, k \rangle\rangle$ indicate nearest neighbor pairs in the same plane and different planes, respectively. The Hamiltonian obeys an essential requirement, i.e., it acts on a subspace of no doubly occupied sites.

To incorporate the coexistence of AF and SC phases, we consider the following variational wave function as the ground state of the Hamiltonian:

$$|\Psi_{var}(\Delta_{sc}, \Delta_{af})\rangle = \mathcal{P}_G \mathcal{P}_N \prod_{\mathbf{k}} (u_{\mathbf{k}} + v_{\mathbf{k}} d_{\mathbf{k}\uparrow}^\dagger d_{-\mathbf{k}\downarrow}^\dagger) |0\rangle, \quad (2)$$

where the operator \mathcal{P}_N projects out the states with a fixed electron number N and $\mathcal{P}_G = \prod_i (1 - n_{i\uparrow} n_{i\downarrow})$ is the Gutzwiller projector which imposes the condition of no double occupancy. The product in Eq. (2) is for over all the \mathbf{k} points in the first Brillouin zone, and the amplitudes $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ are defined by

$$\frac{v_{\mathbf{k}}}{u_{\mathbf{k}}} = \phi(\mathbf{k}) = \frac{\Delta_{\mathbf{k}}}{(\mp E_{\mathbf{k}} - \mu) + \sqrt{(\mp E_{\mathbf{k}} - \mu)^2 + \Delta_{\mathbf{k}}^2}}, \quad (3)$$

where $\Delta_{\mathbf{k}} = \Delta_{sc} f(\mathbf{k})$ represents the SC gap, $f(\mathbf{k})$ being an appropriate symmetry function of \mathbf{k} , and $E_{\mathbf{k}} = \sqrt{\epsilon_{\mathbf{k}}^2 + \Delta_{af}^2}$. $\epsilon_{\mathbf{k}} = -2t(\cos k_x + \cos k_y) - 2t_\perp \cos k_z$ is the free electron dispersion and μ is the chemical potential. The $-$ ($+$) sign in the de-

nominator of Eq. (3) correspond to $\epsilon_{\mathbf{k}} < 0$ ($\epsilon_{\mathbf{k}} > 0$). The quasiparticle operators $d_{\mathbf{k}\sigma}^\dagger$ diagonalize the AF Hartree-Fock Hamiltonian¹⁷ with a gap Δ_{af} and are related to the electron operators by the following transformation:

$$\begin{bmatrix} d_{\mathbf{k}\sigma}^\dagger \\ d_{\mathbf{k}+\mathbf{Q}\sigma}^\dagger \end{bmatrix} = \begin{bmatrix} \alpha_{\mathbf{k}} & \eta(\sigma)\beta_{\mathbf{k}} \\ -\eta(\sigma)\beta_{\mathbf{k}} & \alpha_{\mathbf{k}} \end{bmatrix} \begin{bmatrix} c_{\mathbf{k}\sigma}^\dagger \\ c_{\mathbf{k}+\mathbf{Q}\sigma}^\dagger \end{bmatrix}, \quad (4)$$

with

$$\alpha_{\mathbf{k}} = \frac{1}{\sqrt{2}} \left(1 - \frac{\epsilon_{\mathbf{k}}}{E_{\mathbf{k}}} \right)^{1/2}, \quad \beta_{\mathbf{k}} = \frac{1}{\sqrt{2}} \left(1 + \frac{\epsilon_{\mathbf{k}}}{E_{\mathbf{k}}} \right)^{1/2}. \quad (5)$$

Here, $\mathbf{Q} = (\pi, \pi, \pi)$ is the perfect nesting vector and $\eta(\sigma) = \pm 1$ for $\sigma = \uparrow, \downarrow$.

The wave function in Eq. (2) consists of two variational parameters, viz., Δ_{sc} and Δ_{af} . Ideally, the chemical potential μ should also be treated as a variational parameter; however, here we fix it at its noninteracting value μ_0 . This is because the energy correction obtained by varying μ has been found to be negligibly small (for small J)¹⁶ for a square lattice, and we expect it to be the same also for bilayers. The wave function describes different phases depending on the (relative) values of the variational parameters. For example, $\Delta_{af} = 0$ describes the usual BCS superconducting state,²⁴ whereas in the limit $\Delta_{sc} \rightarrow 0$, the wave function reduces to a state with antiferromagnetic long range order.²⁵ For nonzero Δ_{sc} and Δ_{af} , the wave function describes a phase with coexisting AF and SC states, while the normal state is recovered as both parameters vanish.

III. RESULTS

We shall skip the details of the variational Monte Carlo method used as it appears elsewhere^{23,24,26,34} and only provide the essential features of our computation. We consider periodic boundary condition along the planar x direction and antiperiodic boundary condition in the planar y direction to avoid singularity in $\phi(\mathbf{k})$ for the \mathbf{k} points with $k_x = k_y$ and $\epsilon_{\mathbf{k}} - \mu \leq 0$.²⁴ In one Monte Carlo sweep (MCS) through the lattice, N_s (equal to the number of lattice sites) random moves are attempted, which consist of moving an electron to an empty site and exchanging two antiparallel spins. After each successful move, Monte Carlo updates of the configurations are made by using the inverse update method.²⁷ Various expectation values that are obtained in this paper are computed by sampling configurations chosen from about 10^4 to 10^5 MCSs after taking 5000 warm-up sweeps. Simulations are performed on a bilayered lattice of size $10 \times 10 \times 2$.

In the following, we discuss the stability of different phases with different SC pairing symmetries, followed by the results for magnetic and superconducting correlations. We show that the AF and SC phases coexist in the underdoped regime by comparing the optimal energy of the variational wave function having pure SC correlations with the one having coexisting AF and SC orders. To characterize the pure SC and the coexisting phases and to enumerate the differences in their properties, we compute the correlation functions for both these phases and make a detailed comparison between the two.

A. Stability of different phases

We first consider the pure SC wave function [obtained by putting $\Delta_{af}=0$ in Eq. (2)]. As for the pairing symmetry of the SC state, we considered energies of four different variational wave functions listed in the previous section. An earlier work²³ investigates in detail the first three wave functions in the list and found that the pure d -wave state yields the lowest energy at all values of δ away from half filling. This led to the conclusion that of the three pairing symmetries discussed there, a planar d -wave state is most appropriate in the context of a t - J bilayer. We have included the s^\pm state for comparison with the existing ones in the light of the emphasis given to it where it is claimed to be more stable than that of the d -wave state for the bilayered systems and is capable of explaining the origin of the neutron scattering peak observed experimentally in $\text{YBa}_2\text{Cu}_3\text{O}_7$ at temperatures below T_c .^{18,19,29} However, our VMC calculations indicate the energy of the s^\pm pairing state to be actually higher than the normal state at all values of hole concentrations. Thus, we discard this pairing symmetry from the list of possible candidates and conclude that a planar d -wave state is most appropriate in studying superconductivity in bilayers.

B. Ground state energy

Before we proceed to the calculation of the physical quantities, such as the ground state energy, etc., it is somewhat interesting to look at the variation of the optimal superconducting variational parameter $\tilde{\Delta}_{sc}$ as a function of hole concentration for a few representative values of the interplanar coupling parameters. The choices of these parameters are chosen from experimental data.^{30,31} From Fig. 1, it may be noticed that the critical hole concentration δ_c at which $\tilde{\Delta}_{sc}$ vanishes increases (from ~ 0.3 to ~ 0.34) with larger interplanar hopping t_\perp , while the interplanar exchange J_\perp has no significant effect on δ_c . Below δ_c , $\tilde{\Delta}_{sc}$ is slightly reduced by both higher values of t_\perp and J_\perp . It is worth mentioning here that in a two-dimensional square lattice (with same values for the planar parameters), a d -wave state is stabilized up to $\sim 28\%$ hole concentration,¹⁶ which is lower than the corresponding value i.e., 34% obtained here for the bilayer (Fig. 1). Thus, stability of the superconducting state extends up to *higher* values of hole concentration in bilayers than in planar materials.

Next, we introduce the second variational parameter, i.e., Δ_{af} into the problem and carry out minimization of energy in two-variational-parameter space, Δ_{sc} and Δ_{af} . The calculation shows that the energy is significantly lowered in the underdoped regime ($\delta < 0.14$) when compared to that obtained for the pure SC state. The optimal energy E_{min}/t (per site) as function of δ for the two cases is shown in Fig. 2 for one particular choice for the interplanar parameters. The energy difference between the two phases is maximum at half filling, decreases gradually with increasing hole concentration, and finally vanishing at $\delta \sim 0.14$. Thus, superconductivity coexists with antiferromagnetism in the underdoped region for a bilayer, a feature also observed for the two-dimensional t - J model.¹⁷ This is one of the key results of our

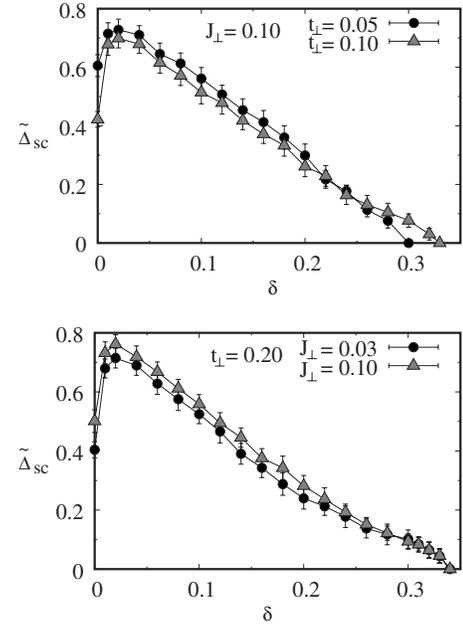


FIG. 1. Optimal value of the variational parameter $\tilde{\Delta}_{sc}$ shown as a function of hole concentration δ corresponding to different choices for the interplanar parameters. All the figures in this paper correspond to calculations done on a lattice size of $10 \times 10 \times 2$. The parameter values are taken in units of (planar) hopping t .

paper. Similar energy differences of the two phases are found for other choices of t_\perp and J_\perp (as shown in Fig. 1).

C. Magnetic order

We first examine the magnetic correlations in the pure d -wave state. The relevant quantities to compute are planar spin-spin correlations $\langle S_i^z S_j^z \rangle$ and the corresponding Fourier transform $S(\mathbf{q})$, called the structure factor, which is defined as

$$S(\mathbf{q}) = \frac{1}{N} \sum_{ij} e^{i\mathbf{q} \cdot (\mathbf{r}_i - \mathbf{r}_j)} \langle S_i^z S_j^z \rangle. \quad (6)$$

The real-space correlations [Fig. 3(a)] show signature of AF order in the planes. However, the correlations are found to decay as a function of planar distances, suggesting an ab-

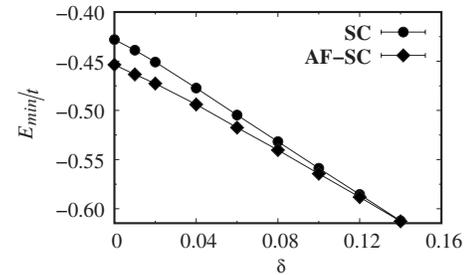


FIG. 2. Optimal energy E_{min}/t (per site) for the pure d -wave SC state and the coexisting AF and SC states as a function of hole concentration δ for $t_\perp = 0.20$ and $J_\perp = 0.10$.

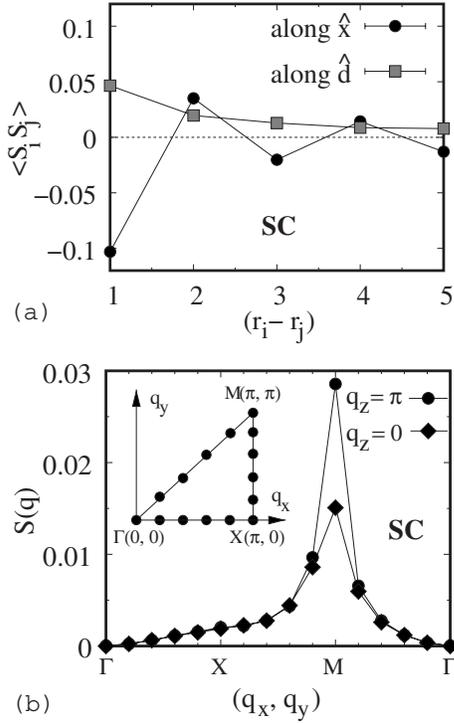


FIG. 3. (a) Spin-spin correlation as a function of distance along a planar edge (\hat{x} direction) and along a planar diagonal (\hat{d} direction). (b) Spin structure factor $S(\mathbf{q})$ as a function of \mathbf{q} chosen along the symmetry lines shown in the figure. The plots shown are at half filling and for $t_{\perp}=0.20$ and $J_{\perp}=0.10$.

sence of antiferromagnetic long range order (AFLRO) even at half filling. It may be noted that the d -wave state does not show long range magnetic order also in two-dimensional systems. As for the interplanar correlations, the d -wave shows AF ordering between the spins in the two layers; however, the correlations are found to be very weak. For instance, the strength of the nearest neighbor spin correlation for two corresponding sites in different planes is approximately 10% of that for two sites in the same plane. In Fig. 3(b), we plot $S(\mathbf{q})$ as a function of (q_x, q_y) , the points being chosen along a symmetry path for q_z equal to both 0 and π . The peak in $S(\mathbf{q})$ at (π, π, π) indicates the existence of antiferromagnetic correlations in the lattice. However, the peak at $(\pi, \pi, 0)$ is of comparable magnitude to that at (π, π, π) , which corroborates the presence of weak interplanar correlations mentioned earlier.²⁸ Away from half filling, both planar and interplanar spin correlations are found to vanish rapidly with hole doping. Other values for the interplanar parameters among the ones considered here are found to have little impact on spin correlations except for a small reduction of planar correlations by larger interplanar hopping away from half filling. The value of staggered structure factor $S(\pi, \pi, \pi)$ at half filling for the d -wave state is obtained as ~ 0.03 . This value may be compared with the exact diagonalization results for a bilayer t - J model,³² which yields an estimate for $S(\pi, \pi, \pi)$ to be ~ 0.45 for $J_{\perp}/J \approx 0.28$ (the same corresponding value is used in Fig. 3) at half filling.³³ Thus, the staggered magnetization for the pure d -wave state obtained in our calculations is far lower than that obtained via exact

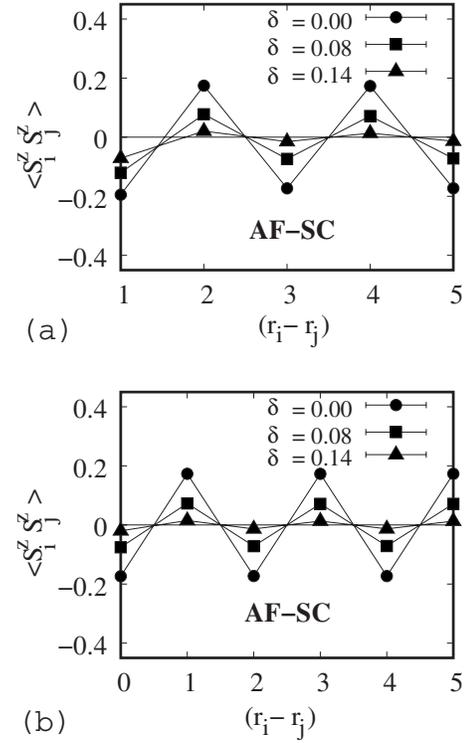


FIG. 4. Spin-spin correlation as a function of distance along the \hat{x} direction for the coexisting AF and d -wave SC (AF-SC) states. The spins are on lattice sites lying (a) along an edge in a plane and (b) on two different planes along the same direction. The values of the hole concentration δ are shown in the figures. Here, the interplanar parameters are again chosen as $t_{\perp}=0.20$ and $J_{\perp}=0.10$.

diagonalization studies. This large discrepancy can be attributed mainly to the absence of interlayer magnetic correlations for the pure d -wave state.

Next, we discuss the magnetic correlations in the coexisting AF and d -wave SC state, which is lower in energy than that of the pure d -wave SC state in the underdoped region. In Fig. 4, we show the planar and interplanar spin correlations both at and away from half filling. The correlations are clearly much stronger in this case than for the pure d -wave state. The interplanar correlations, which were very weak in the d -wave state, are almost of the same magnitude as the planar correlations. In addition, the magnitude of correlations does not seem to decay with distance at and even slightly away from half filling. However, at larger values of δ , the magnetic correlations decay rapidly with distance as seen for $\delta=0.14$ in Fig. 4. The energy calculations also provide support for this result, where it is found that the kinetic energy dominates over the exchange energy and, consequently, the antiferromagnetic phase disappears corresponding to $\delta \sim 0.14$. The presence of magnetic order in the coexisting phase is further emphasized by plotting $S(\mathbf{q})$ versus \mathbf{q} at various hole concentrations in Fig. 5. The sharp peaks in $S(\mathbf{q})$ at $\mathbf{q}=(\pi, \pi, \pi)$ for small values of hole doping [Fig. 5(a)] indicate the existence of strong AF long range correlations in the system. It should be noted that the value of $S(\pi, \pi, \pi)$ at half filling is ~ 0.35 , which is considerably larger than that obtained for the pure SC state and is compa-

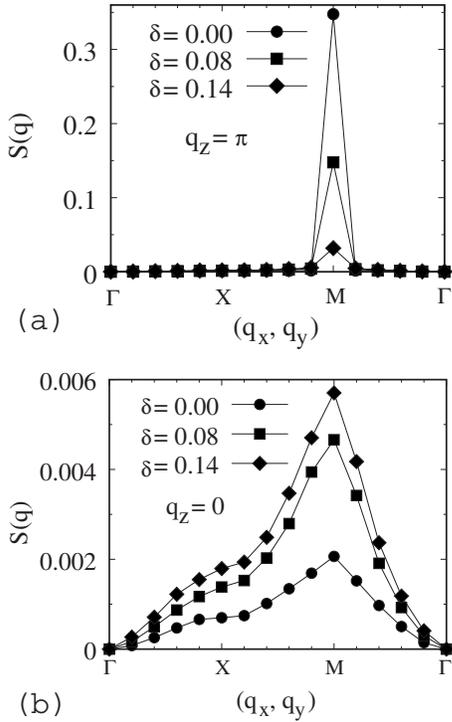


FIG. 5. $S(\mathbf{q})$ as a function of \mathbf{q} for the AF-SC wave function at various hole concentrations shown in the figure. The (q_x, q_y) points are chosen in the same way as in Fig. 3(b). $t_{\perp} = 0.20$ and $J_{\perp} = 0.10$.

erable to the exact diagonalization value (viz., 0.45) mentioned earlier.³² Thus, the support for the coexisting phase becomes more robust. Also, $S(\pi, \pi, \pi)$ decreases with increasing hole concentration as the magnetic correlations are weakened by the mobile holes. For $q_z = 0$ [Fig. 5(b)], it is observed that $S(\mathbf{q})$ increases with increasing hole concentration, the increase being maximum at $(\pi, \pi, 0)$. This signals rapid suppression of interplanar AF long range correlations away from half filling.

Next, we incorporate the effect of interplanar couplings on the magnetic correlations. Figure 6 shows the variations of $S(\pi, \pi, \pi)$ and $S(\pi, \pi, 0)$ with t_{\perp} and J_{\perp} both at and away from half filling. In Figs. 6(a) and 6(b), we let t_{\perp} vary while keeping J_{\perp} constant. It is seen that t_{\perp} has no effect on magnetic correlations at half filling, which is expected as hopping of electron is forbidden at half filling due to the no double occupancy constraint. Away from half filling, $S(\pi, \pi, \pi)$ shows a decrease with increasing t_{\perp} , thus indicating that AFLRO diminishes by larger interplanar hopping. Further, the decrease of $S(\pi, \pi, 0)$ with increasing t_{\perp} implies that the planar correlations are mainly affected. On the other hand, variation of interplanar exchange is found to have the reverse effect on the correlations. Figure 6(c) shows that $S(\pi, \pi, \pi)$ increases with larger J_{\perp} both at and away from half filling. However, $S(\pi, \pi, 0)$ [Fig. 6(d)] decreases with increasing J_{\perp} . This is a reflection of the fact that interplanar AF correlations are strengthened by larger J_{\perp} , while the planar correlations are almost unaffected. This agrees with exact diagonalization results obtained for the bilayer t - J model.³² Thus, we conclude that larger t_{\perp} reduces planar magnetic correlations away from half filling, while larger J_{\perp} enhances

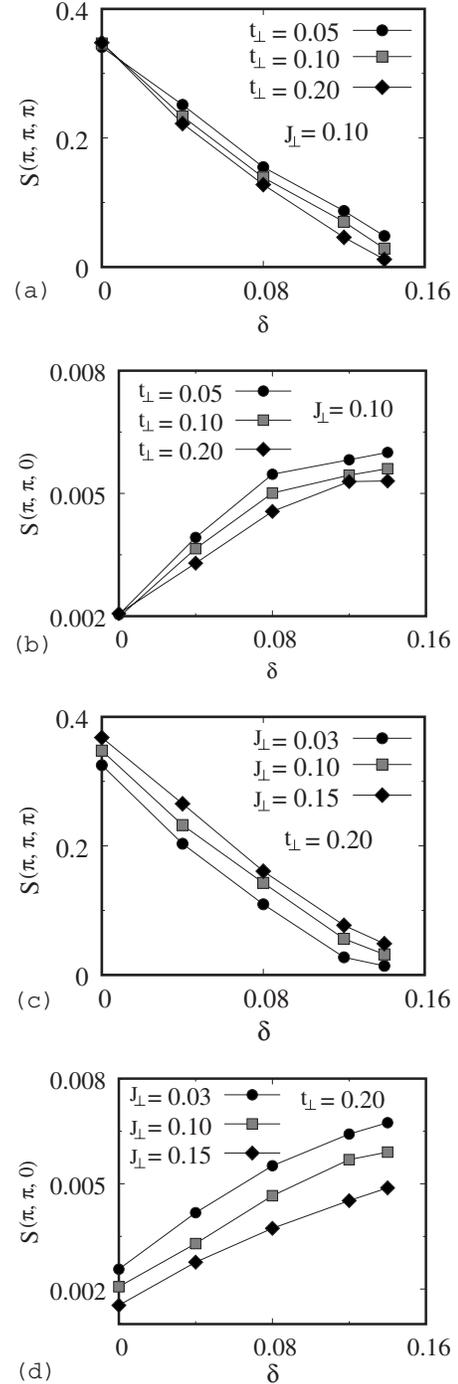


FIG. 6. $S(\pi, \pi, \pi)$ and $S(\pi, \pi, 0)$ are plotted as a function of hole concentration for various values of interplanar parameters shown in the figure, showing the effect of interplanar couplings on the AF long range order for the AF-SC state. (a) and (b) involve variation of t_{\perp} for a fixed J_{\perp} , and (c) and (d) contain variation of J_{\perp} for a fixed t_{\perp} .

interplanar correlations both at and away from half filling.

D. Superconducting correlations

Our next job constitutes investigating SC correlations for both pure SC and coexisting AF and SC states. The SC correlation function is defined as

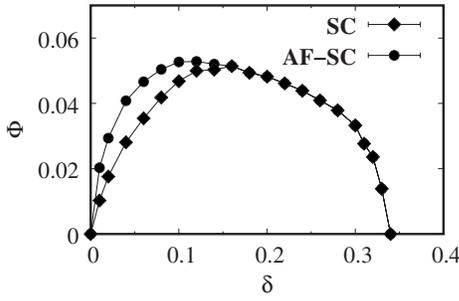


FIG. 7. SC order parameter Φ shown as a function of hole concentration δ for the AF-SC and pure SC states. Here, the interplanar parameters are chosen as $t_{\perp}=0.20$ and $J_{\perp}=0.10$.

$$F_{\alpha,\beta}(\mathbf{r}-\mathbf{r}') = \langle B_{\mathbf{r}\alpha}^{\dagger} B_{\mathbf{r}'\beta} \rangle, \quad (7)$$

where B 's are pair operators and are represented by $B_{\mathbf{r}\beta} = \frac{1}{2}(c_{\mathbf{r}'\uparrow}c_{\mathbf{r}'+\beta\downarrow} - c_{\mathbf{r}'\downarrow}c_{\mathbf{r}'+\beta\uparrow})$, which annihilates a singlet pair on bond $(\mathbf{r}', \mathbf{r}'+\beta)$, and $B_{\mathbf{r}\alpha}^{\dagger}$ creates one on $(\mathbf{r}, \mathbf{r}+\alpha)$. α and β are unit vectors connecting to nearest neighbors in the x , y (planar) and z (across the plane) directions. We have computed $F_{\alpha,\beta}$ as a function of distance $|\mathbf{r}-\mathbf{r}'|$ for different hole concentrations corresponding to several choices for the interplanar parameters. A very useful quantity in this connection is the SC order parameter Φ , which is obtained as²⁴ $F_{\alpha,\beta}(\mathbf{r}-\mathbf{r}') \rightarrow \pm\Phi^2$ for large $|\mathbf{r}-\mathbf{r}'|$, with the sign being $+$ ($-$) for α to be \parallel (\perp) to β (both α and β lie on a single layer).

To examine interplanar SC correlations, we have calculated $F_{\alpha,\beta}(\mathbf{r}-\mathbf{r}')$ taking both α and β to be along z direction. The values obtained at all hole concentrations are very small (smaller than the error bars), i.e., negligible in comparison to the planar correlation values. The result appears as no surprise as the pure d -wave state, which is found to most suitably describe pairing symmetry for a bilayer, contains no significant interplanar SC correlations.

Next, we show that the planar SC correlations are stronger in the AF-SC state in the region of hole doping (i.e., underdoped) in which the two phases coexist in comparison to that in the pure SC state. Figure 7 shows the SC order parameter Φ corresponding to planar $F_{\alpha,\beta}(\mathbf{r}-\mathbf{r}')$ [i.e., (α, β) along (x, y) as function of δ for both the pure SC and the AF-SC states]. The figure clearly shows that SC correlations are stronger in the coexisting phase than in the pure SC state. It is very interesting to note that the coexisting phase, which is energetically favorable in the underdoped region, gives rise to not only *stronger AF correlations* but also *enhanced SC correlations* as compared to that in pure SC state. This is another important result of our paper.

Next, to estimate the effects of interplanar couplings on the SC correlations in a plane, we calculate the SC order parameter Φ as a function of hole concentrations for different choices of t_{\perp} and J_{\perp} . The results are shown in Fig. 8 with t_{\perp} varying from 0.05 to 0.2 and $J_{\perp}=0.1$. From the figure, one observes that the SC correlations vary significantly and differently in the optimally doped and the overdoped regimes with the interplanar hopping t_{\perp} . In the underdoped region, the effect of t_{\perp} is small. At optimal values of doping, i.e., in

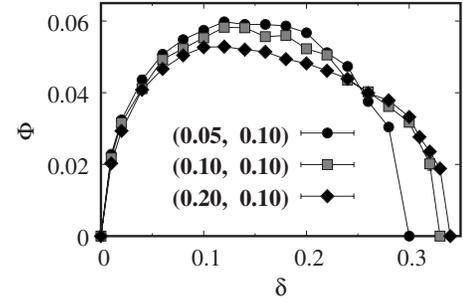


FIG. 8. SC order parameter Φ versus hole concentration δ for different values of t_{\perp} with $J_{\perp}=0.1$. The numbers in parentheses shown in figure are the values of (t_{\perp}, J_{\perp}) .

the peak region of order parameter Φ , larger interplanar hopping reduces planar SC correlations strongly. However, just the opposite behavior is observed in the overdoped region. As shown in Fig. 8, for $t_{\perp}=0.05$, the optimally doped region is marked by largest Φ , indicating greater stability of the SC state for smaller t_{\perp} . The critical hole concentration δ_c , at which the phase transition from SC to normal state takes place, is ~ 0.30 for $t_{\perp}=0.05$, while for $t_{\perp}=0.10$ and 0.20 , δ_c 's are obtained as 0.33 and 0.34 , respectively. Thus, increasing the interlayer hopping in a bilayer results in greater stability of the SC state in the overdoped region. With regard to the impact due to interplanar exchange J_{\perp} , our calculations show that J_{\perp} has no perceptible effect (figures not shown here) on the SC correlations at least for the values of J_{\perp} considered here.

The asymmetric behavior shown by superconducting correlations in the optimally doped and the overdoped regime as t_{\perp} is increased from 0.05 to 0.20 constitutes another key finding of this paper. While the reduction of planar SC correlations with increasing t_{\perp} as observed in optimally doped region is expected due to the fact that larger hoppings have a disrupting effect on the pairing, the reason for the opposite behavior in the overdoped regime where SC correlations are enhanced by larger t_{\perp} is not immediately obvious. To explain this, we look at momentum distribution for two different values of t_{\perp} , viz., 0.05 and 0.20. Figure 9 shows the 2D projection of momentum distribution function $n(\mathbf{k}) = \langle c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}\sigma} \rangle$, for $\delta=0.32$. At this hole doping value, there is a large variation in SC order parameter for the two values of t_{\perp} (actually, SC order is vanishing small at $\delta=0.32$ for $t_{\perp}=0.05$). It is seen from the plots that there is a significant variation of $n(\mathbf{k})$ weights in the two momentum planes, viz., the $k_z=0$ and $k_z=\pi$, as t_{\perp} is varied. The spectral weight shifts from the $k_z=\pi$ plane to the $k_z=0$ plane as t_{\perp} is increased from 0.05 to 0.20. Thus, for larger t_{\perp} , occupation of the pairs with $k_z=0$ is higher in the overdoped region. This favors the stability of SC phase as the $k_z=0$ pairs are planar and contribute in the development of the SC order. The $k_z=\pi$ pairs are interplanar and hence are not expected to be key players as the SC correlations are essentially planar. We believe that this transfer of weight from $k_z=\pi$ to $k_z=0$ for larger t_{\perp} helps in stabilizing the SC order in the overdoped region even though the disrupting effect due to larger interplanar hopping persists. In the optimally doped region, the momentum dis-

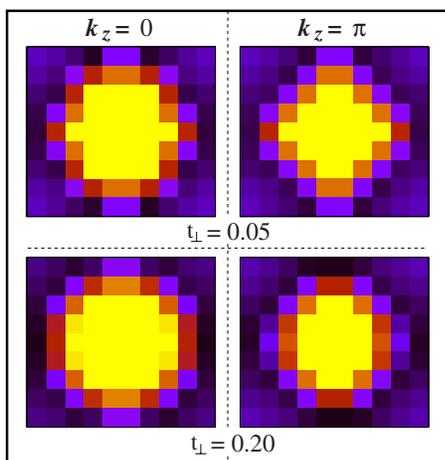


FIG. 9. (Color online) Plots of $n(\mathbf{k})$ projected on a two-dimensional (k_x, k_y) plane where white (yellow) and gray (magenta) colors represent the highest and lowest spectral weights, respectively. The left panel shows $n(k)$ for $k_z=0$ and the right panel corresponds to $k_z=\pi$, for $t_{\perp}=0.05$ (top) and 0.20 (bottom). The hole concentration here is $\delta=0.32$.

tribution profiles for different values of t_{\perp} are found to be almost identical (plots not shown here) and hence the only effect of t_{\perp} is to reduce the SC correlations.

Regarding the finite size effects in our results, we would like to mention here that the magnitudes of various quantities calculated do show some dependence on the size of the lattice. The dependence of energy on lattice size is elucidated in detail in Ref. 23. However, the main features of the key results here, e.g., the coexistence of AF and SC orders, the effect of interlayer parameters on the properties, etc., will remain qualitatively the same with lattice size.

IV. CONCLUSION

We summarize our main results obtained using variational calculations for a t - J bilayer as follows: Coexisting AF-SC state is found to be more stable than the pure (d -wave) SC state at low values of doping ($\delta < 0.14$). Beyond this, of course, the SC state is found to have the lowest energy and remains stable up to a hole concentration that is more than that obtained for a two-dimensional square lattice. Further, a detailed analysis of magnetic and superconducting properties yields the coexisting phase, which is not only energetically stable but also supports a stronger AF and SC correlations. The third and possibly the most important result emerges when the effects of interplanar coupling parameters are invoked for discussion, and it appears in the form of an asymmetry in the optimally and the overdoped region where the planar SC correlations are found to be more stable for smaller and larger interplanar hoppings, respectively. However, the interplanar exchange does not play a decisive role in SC correlations.

Some of the other results obtained by us include a comparison of the nature of magnetic correlations between the pure SC state and the AF-SC state. It is found that strong planar and interplanar AF correlations exist in the AF-SC state at and slightly away from half filling, whereas in the pure SC state, the magnetic correlations are very weak. We have also discussed the effects of interplanar coupling on magnetic correlations in the AF-SC state, where larger t_{\perp} reduces planar magnetic correlations whereas larger J_{\perp} enhances interplanar magnetic correlations.

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