

## Absence of the coexistence of superconductivity and antiferromagnetism in the hole-doped two-dimensional extended $t$ - $J$ model

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The possibility of coexistence of superconductivity (SC) and antiferromagnetic long-range order (AFLRO) of the two-dimensional extended  $t$ - $J$  model in the very underdoped region is studied by the variational Monte Carlo (VMC) method. In addition to using previously studied wave functions, a recently proposed wave function generated from the half-filled Mott insulator is used. For hole-doped systems, the phase boundary between AFLRO and  $d$ -wave SC for the physical parameters,  $J/t=0.3$ ,  $t'/t=-0.3$  and  $t''/t=0.2$ , is located near hole density  $\delta_c \cong 0.06$ , and there is *no* coexistence. The phase transition is first order between these two homogeneous phases at  $\delta_c$ .

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Correlation between the  $d$ -wave SC and AFLRO is one of the critical issues in the physics of the high-temperature superconductivity (HTS).<sup>1,2</sup> Early experimental results showed one of the common features of the HTS cuprates is the existence of AFLRO at temperature lower than the Néel temperature  $T_N$  in the insulating perovskite parent compounds. When charge carriers (electrons or holes) are doped into the parent compounds, AFLRO is destroyed quickly and then SC appears. In most thermodynamic measurements, AFLRO does not coexist with SC.<sup>3</sup> However, this is still a controversial issue. Recent experiments such as neutron-scattering and muon spin rotation show that the spin density wave (SDW) may compete, or coexist with SC under the external magnetic field.<sup>4-6</sup> Remarkably, elastic neutron scattering experiments for underdoped  $\text{YBa}_2\text{Cu}_3\text{O}_x$  ( $x=6.5$  and  $6.6$ ,  $T_c=55$  K and  $62.7$  K, respectively) show that the commensurate AFLRO develops around room temperature with a large correlation length  $\sim 100$  Å and a small staggered magnetization  $m_0 \sim 0.05 \mu_B$ .<sup>7-9</sup> These results suggest that AFLRO may coexist with SC but the possibility of inhomogeneous phases is not completely ruled out.

For the theoretical part, the two-dimensional (2D)  $t$ - $J$  model is proposed<sup>10</sup> to understand the physics of HTS. Anderson proposed the resonating-valence-bond (RVB) theory for the model about one and a half decades ago. The theory is reexamined again<sup>11</sup> recently. The authors compared the prediction of the RVB theory with several experimental results and found the theory to have successfully explained the main features of cuprates. This so called “plain vanilla” theory did not consider the issue of AFLRO, which must be addressed at very low doping. From analytical and numerical studies of the  $t$ - $J$  model, it was shown that at half-filling, the  $d$ -wave RVB state with AFLRO is a good trial wave function (TWF). In this case, SC correlation is zero because of the constraint of no-double-occupancy. Upon doping, the carriers become mobile and SC revives while AFLRO is quickly suppressed. However, if the doping density is still small, AFLRO will survive. Thus SC and AFLRO coexist in the very underdoped regime.<sup>12-16</sup> Exact diagonalization (ED) up

to 26 sites show that both SC and AFLRO are enhanced by the external staggered field. This result also implies these two orders can coexist homogeneously in a 2D  $t$ - $J$  model.<sup>17</sup> However, the regime of AFLRO predicted by these studies extend to larger doping than the experimental results. The robustness of the coexistence of SC and AFLRO seems to be inconsistent with experiments.<sup>18</sup>

There are several experimental and theoretical studies suggesting the presence of the next- and third-nearest-neighbor hopping terms  $t'$  and  $t''$  in cuprates. For example, the topology of the large Fermi surface and the single-hole dispersion studied by ARPES,<sup>19</sup> and the asymmetry of phase diagrams of the electron- and hole-doped cuprates can be understood by introducing these terms. Further, these longer range hopping terms may be essential for the large enough  $T_c$  for the  $t$ - $J$ -type models.<sup>20,21</sup> In this paper, we would like to demonstrate the phase diagram constructed by VMC results of the extended  $t$ - $J$  model. The TWF's for very underdoped systems are generalized from the single-hole and slightly doped wave function (WF) proposed by Lee *et al.*<sup>22,23</sup> The results for the hole-doped case show there is *no* coexistence of  $d$ -wave pairing and AFLRO when the next- and third-nearest neighbor hopping terms are introduced. And the phase boundary of AFLRO is pushed to lower doping density.

The Hamiltonian of the extended  $t$ - $J$  model is

$$H = H_t + H_J = - \sum_{ij} t_{ij} (\tilde{c}_{i,\sigma}^\dagger \tilde{c}_{j,\sigma} + \text{H.C.}) + J \sum_{\langle i,j \rangle} \left( \mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4} n_i n_j \right) \quad (1)$$

where  $t_{ij}=t$ ,  $t'$ , and  $t''$  for sites  $i$  and  $j$  are nearest, next-nearest, and the third-nearest neighbors.  $\langle i,j \rangle$  in  $H_J$  means the spin-spin interaction occurs only for nearest neighbors.  $\tilde{c}_{i,\sigma} = (1 - n_{i,-\sigma}) c_{i,\sigma}$ , satisfies the no-double-occupancy constraint. At half-filling, the system is reduced to the Heisenberg Hamiltonian  $H_J$ . As carriers are doped into the parent compound,  $H_t$  is included in the Hamiltonian.

First we exam the phase diagram of the  $t$ - $J$  model, that is,  $t' = t'' = 0$ . Following Refs. 15 and 22, three mean-field order parameters are introduced: the staggered magnetization  $m_s = \langle S_A^z \rangle = -\langle S_B^z \rangle$ , where the lattice is divided into  $A$  and  $B$  sublattices, the uniform bond order parameters  $\chi = \langle \sum_{\sigma} c_{i\sigma}^\dagger c_{j\sigma} \rangle$ , and  $d$ -wave RVB ( $d$ -RVB) one  $\Delta = \langle c_{j\downarrow} c_{i\uparrow} - c_{j\uparrow} c_{i\downarrow} \rangle$  if  $i$  and  $j$  are nearest-neighbor sites in the  $x$  direction and  $-\Delta$  for the  $y$  direction. The Lee-Shih WF, which is the mean-field ground state WF, is

$$|\Psi_{LS}\rangle = P_d \left( \sum_{\mathbf{k} \in SBZ} (A_{\mathbf{k}} a_{\mathbf{k}\uparrow}^\dagger a_{-\mathbf{k}\downarrow}^\dagger + B_{\mathbf{k}} b_{\mathbf{k}\uparrow}^\dagger b_{-\mathbf{k}\downarrow}^\dagger) \right)^{N_s/2} |0\rangle, \quad (2)$$

where  $N_s$  is the total number of sites and  $A_{\mathbf{k}} = (E_{\mathbf{k}}^{(1)} + \xi_{\mathbf{k}}^-) / \Delta_{\mathbf{k}}$  and  $B_{\mathbf{k}} = -(E_{\mathbf{k}}^{(2)} - \xi_{\mathbf{k}}^+) / \Delta_{\mathbf{k}}$  with  $E_{\mathbf{k}}^{(1)} = (\xi_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2)^{1/2}$  and  $E_{\mathbf{k}}^{(2)} = (\xi_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2)^{1/2}$ . Here  $\Delta_{\mathbf{k}} = \frac{3}{4} \Delta (\cos k_x - \cos k_y)$ . Energy dispersions for the two SDW bands are  $\xi_{\mathbf{k}}^\pm = \pm [(\epsilon_{\mathbf{k}} + \mu)^2 + (Jm_s)^2]^{1/2} - \mu$  with  $\epsilon_{\mathbf{k}} = -2(t\delta + \frac{3}{8}J\chi)(\cos k_x + \cos k_y)$ .  $a_{\mathbf{k}\sigma} = \alpha_{\mathbf{k}} c_{\mathbf{k}\sigma} + \sigma \beta_{\mathbf{k}} c_{\mathbf{k}+\mathbf{Q}\sigma}$  and  $b_{\mathbf{k}\sigma} = -\sigma \beta_{\mathbf{k}} c_{\mathbf{k}\sigma} + \alpha_{\mathbf{k}} c_{\mathbf{k}+\mathbf{Q}\sigma}$ , where  $\mathbf{Q} = (\pi, \pi)$ ,  $\alpha_{\mathbf{k}}^2 = \frac{1}{2} \{1 - [(\epsilon_{\mathbf{k}} + \mu) / (\xi_{\mathbf{k}}^+ + \mu)]\}$ , and  $\beta_{\mathbf{k}}^2 = \frac{1}{2} \{1 + [(\epsilon_{\mathbf{k}} + \mu) / (\xi_{\mathbf{k}}^+ + \mu)]\}$  are the operators of the lower and upper SDW bands, respectively.  $\mu$  is the chemical potential which determines the number of electrons. Note that the summation in Eq. (2) is taken over the sublattice Brillouin zone (SBZ). The operator  $P_d$  enforces the constraint of no doubly occupied sites for cases with finite doping.

For the half-filled case,  $\mu = 0$  and the optimal variational energy of this TWF obtained by tuning  $\Delta$  and  $m_s$  in the VMC simulation is  $-0.332J$  per bond which is within 1% of the best estimate of the ground state energy of the Heisenberg model. For the case of pure AFLRO without  $\Delta$ , energy per bond is about 3% to 4% higher. Upon doping, there are two methods to modify the TWF: one is to use the SDW bands with a nonzero  $\mu$ , the other is to create charge excitations from the half-filled ground states. For the former method, the TWF is optimized by tuning  $\Delta$ ,  $m_s$  and  $\mu$ . Note that for larger doping densities, AFLRO disappears ( $m_s = 0$ ) and the WF reduces to the standard  $d$ -RVB WF. For the latter method, the WF is the ‘‘small Fermi pocket’’ state  $|\Psi_p\rangle$ :

$$|\Psi_p\rangle = P_d \left( \sum_{\mathbf{k} \in SBZ, \mathbf{k} \in Q_p} (A_{\mathbf{k}} a_{\mathbf{k}\uparrow}^\dagger a_{-\mathbf{k}\downarrow}^\dagger + B_{\mathbf{k}} b_{\mathbf{k}\uparrow}^\dagger b_{-\mathbf{k}\downarrow}^\dagger) \right)^{N_s/2} |0\rangle. \quad (3)$$

$\mathbf{k} \in Q_p$  means the  $\mathbf{k}$  points in the Fermi pocket  $Q_p$  are not occupied. For example, for four holes in  $12 \times 12$  lattice,  $Q_p = \{(\pi/2, \pi/2), (\pi/2, -\pi/2)\}$ . The number of holes is twice of the number of  $\mathbf{k}$  points in  $Q_p$  and  $\mu$  is identical to zero in Eq. (3). In general, for the ground state the set  $Q_p$  should be determined variationally. Yet as we expected, it agrees well with the rigid band picture shown in Ref. 23.

The staggered magnetization  $\langle M \rangle = (1/N_s) \langle \sum_j e^{i\mathbf{Q} \cdot \mathbf{R}_j} S_{\mathbf{R}_j}^z \rangle$  and the  $d$ -wave pair-pair correlation  $P_d(\mathbf{R}) = (1/N_s) \langle \sum_i \Delta_{\mathbf{R}_i}^\dagger \Delta_{\mathbf{R}_i + \mathbf{R}} \rangle$ , where  $\Delta_{\mathbf{R}_i} = c_{\mathbf{R}_i\uparrow} (c_{\mathbf{R}_i+\hat{x}\downarrow} + c_{\mathbf{R}_i-\hat{x}\downarrow} - c_{\mathbf{R}_i+\hat{y}\downarrow} - c_{\mathbf{R}_i-\hat{y}\downarrow})$  are measured for  $J/t = 0.3$  and  $t' = t'' = 0$  for the  $12 \times 12$  lattice with periodic boundary condition.  $P_d^{ave}$  is the averaged value of the long-range part ( $|\mathbf{R}| > 2$ ) of  $P_d(\mathbf{R})$ . The resulting  $\langle M \rangle$  (full circles) and  $P_d^{ave}$  (empty circles) are shown in Fig. 1.

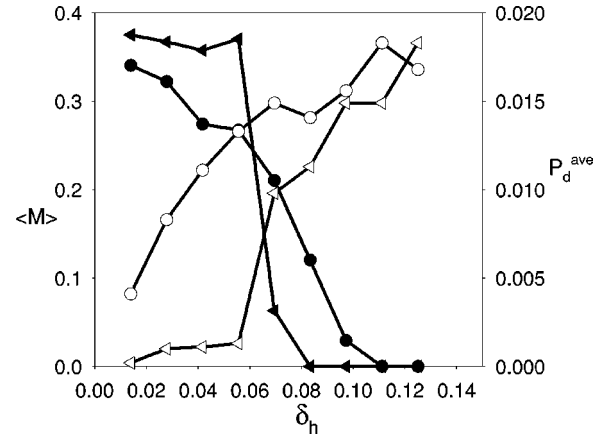


FIG. 1.  $\langle M \rangle$  (full symbols) and  $P_d^{ave}$  (empty symbols) for  $J/t = 0.3$ ,  $t' = t'' = 0$  (circles) and  $t'/t = -0.3$ ,  $t''/t = 0.2$  (triangles) for hole-doped  $12 \times 12$  lattice.

It can be seen in Fig. 1 that in the underdoped region for the  $J/t = 0.3$ ,  $t' = t'' = 0$  case, AFLRO (full circles) coexists with SC (open circles) for  $\delta_c \leq 10\%$ , which is smaller than the weak-coupling mean-field result  $\sim 15\%$ ,<sup>15</sup> but still larger than the phase boundary of AFLRO determined by experiments  $\delta_c < 5\%$ . The energies of  $|\Psi_{LS}\rangle$  are lower than those of  $|\Psi_p\rangle$  for all doping densities in this case. This result is also consistent with the results reported by Himeda and Ogata.<sup>16</sup> Comparison of the VMC result with that of the weak-coupling one seems to indicate that the rigorous no-double-occupancy constraint suppresses the AFLRO faster than the constraint-relaxed mean-field approximation.

Now we examine the phase diagram for  $J/t = 0.3$ ,  $t'/t = -0.3$  and  $t''/t = 0.2$ . For this case, the WF Eq. (2) is modified by replacing  $\mu$  by  $\mu + 4t'_v \cos k_x \cos k_y + 2t''_v (\cos 2k_x + \cos 2k_y)$  due to the second- and third-nearest-neighbor hopping terms.  $t'_v$  and  $t''_v$  are variational parameters.  $t'_v$  and  $t''_v$  are not necessarily equal to the bare values  $t'$  and  $t''$  because the constraint strongly renormalizes the hopping amplitude. On the other hand, the effect of  $t'$  and  $t''$  on  $|\Psi_p\rangle$  is the choice of  $\mathbf{k}$  points in  $Q_p$ , and the form of Eq. (3) is not changed.

The optimal wave functions for different densities are determined by minimizing the variational energies among  $|\Psi_p(m_s, \Delta, \{Q_p\})\rangle$  and  $|\Psi_{LS}(m_s, \Delta, t'_v, t''_v, \mu)\rangle$ . The differences of the energies of best  $|\Psi_p\rangle$  and  $|\Psi_{LS}\rangle$  for various hole densities are shown in Fig. 2.  $\langle M \rangle$  (full triangles) and  $P_d^{ave}$  (open triangles) for  $12 \times 12$  lattice are shown in Fig. 1.

It can be seen that level crossing occurs at  $\delta_h \sim 0.06$ .  $|\Psi_p\rangle$  has lower energy below the critical density. To show  $|\Psi_{LS}\rangle$  and  $|\Psi_p\rangle$  belong to two different types of WF, we calculate the overlap of them.  $(\langle \Psi_{LS} | \Psi_p \rangle / \langle \Psi_{LS} | \Psi_{LS} \rangle \langle \Psi_p | \Psi_p \rangle)$  is only 0.0113(4). The almost orthogonality of the two wave functions implies that the ground state WF's switch at the critical density. Another evidence is shown by the correlation functions of the two wave functions shown in Fig. 3. It is clear that the holes in  $|\Psi_p\rangle$  repel each other and pairing is very small, while the behavior is opposite for  $|\Psi_{LS}\rangle$ .

For  $\delta_h < 0.06$ ,  $|\Psi_p\rangle$  is the ground state WF and  $\langle M \rangle$  is a little larger than the  $t' = t'' = 0$  case while  $P_d^{ave}$  is suppressed

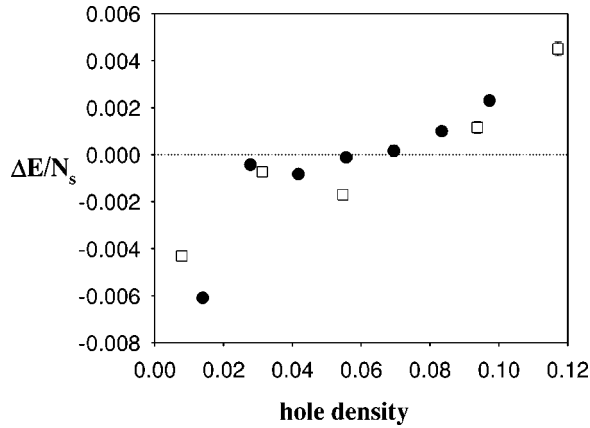


FIG. 2. Energy difference per site between the two wave functions  $|\Psi_p\rangle$  and  $|\Psi_{LS}\rangle$  for  $t'/t=-0.3$  and  $t''/t=0.2$  in  $12 \times 12$  (full circles) and  $16 \times 16$  (open squares) lattices.

by one order of magnitude. Thus there is AFLRO but *no* SC in this regime. The behavior is quite different from  $|\Psi_{LS}\rangle$  for the same doping regime for  $t'=t''=0$  case, whose  $P_d^{ave}$  coexists with  $\langle M \rangle$ . A possible reason for this difference is that although WF  $|\Psi_p\rangle$  gains energy (short-range effect) from its  $d$ -RVB feature the same as  $|\Psi_{LS}\rangle$ , yet  $P_d^{ave}$  is greatly suppressed by replacing the large Fermi surface by the small pocket. This replacement seems to make the WF decoherent for pairing.

For  $\delta_h$  larger than 0.06, the RVB state ( $m_s=0$  in  $|\Psi_{LS}\rangle$ ) optimizes the energy.  $P_d^{ave}$  increases and  $\langle M \rangle$  drops to zero sharply. Unlike the  $t'=t''=0$  case there is no region optimized by  $|\Psi_{LS}\rangle$  with nonzero  $m_s$ . In conclusion, there is no coexistence of AFLRO and SC for the  $t'/t=-0.3, t''/t=0.2$  case. These parameters are close to the values for YBCO and BSCO compounds.<sup>24</sup>

The result that the critical  $\delta_h$  for negative  $t'/t$  is smaller than that of  $t'=0$  case is consistent with the results evaluated by exact diagonalization<sup>25,26</sup> and the suppression of coexistence of AFLRO and SC is consistent with the slave-boson mean-field theory.<sup>27</sup>

The derivation of the effective Hamiltonian of the Hubbard model in the  $U/t \rightarrow \infty$  limit will generate a three-site correlated hopping term  $t_3$  as well as the  $t$ - $J$  terms in Eq. (2).<sup>28,29</sup> Previous studies show that this term enhances SC.<sup>30-33</sup> Since  $t_3$  has a similar extended feature as the  $t'$  term, we have also examined its effect for the AFLRO/SC phase transition. Our VMC results show that the  $t$ - $t_3$ - $J$  model gives similar results as  $t$ - $J$  model for the relevant density regime. Also the shape of Fermi surface is not changed by  $t_3$ .<sup>34</sup> Hence  $t_3$  is not as important as  $t'$ .

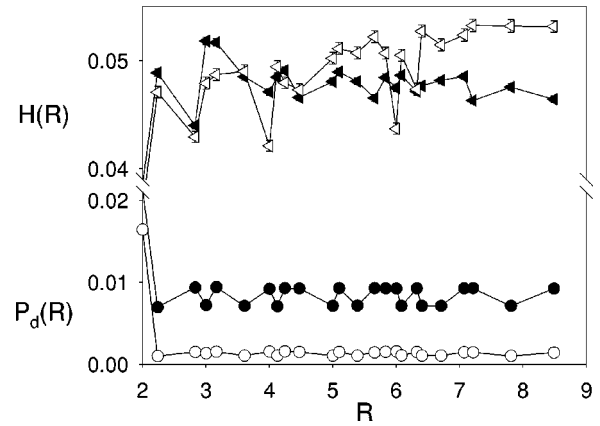


FIG. 3. Pair-pair correlation  $P_d(R)$  (circles) and hole-hole correlation  $H(R)$  (triangles) of  $|\Psi_{LS}\rangle$  (full symbols) and  $|\Psi_p\rangle$  (open symbols) for eight holes in a  $12 \times 12$  lattice.

In summary, for the extended  $t$ - $J$  model, we proposed a new WF  $|\Psi_p\rangle$  for the underdoped regime which has lower variational energy than the traditional WF with coexisting AFLRO and SC. This WF is constructed under the framework of RVB. The new wave function has AFLRO but SC is largely suppressed and there is no coexistence of AFLRO and SC in the underdoped regime of the hole-doped extended  $t$ - $J$  model. The variational phase diagram shows better agreement with experimental results for the underdoped HTS cuprates.

Note that in this study we only consider the homogeneous states. Since the phase transition comes from the level crossing of the two classes of states at the critical density  $\delta_c = 0.06$ , it is a first order phase transition. It is quite natural to have inhomogeneity in the system near the critical point.<sup>35</sup> It may also lead to other more novel inhomogeneous states such as stripe phase.<sup>36</sup> Another interesting result of our study is that the non-coexistence of SC and AFLRO is much more robust for systems with larger values of  $t'/t$  and  $t''/t$  such as YBCO and BSCO.<sup>24</sup> For LSCO where  $t'/t$  and  $t''/t$  are smaller, the tendency toward coexistence is larger and the possibility of inhomogeneous phase will become much more likely.

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