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Mechanism of formation of half-doped stripes in underdoped cuprates

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Using a variational Monte Carlo approach with a recently proposed stripe wave function, we showed that the strong correlation included in a *t*-*J*-type model has essentially all the necessary ingredients to form these stripes with modulations of charge density, spin magnetization, and pair field. If a perturbative effect of electron-phonon coupling to renormalize the effective mass or the hopping rate of holes is considered with the model, we find the half-doped stripes, which has on the average one half of a hole in one period of charge modulation, to be most stable energetic wise in the underdoped region, $1/12 \leq \delta \leq 1/8$. This is in good agreement with the observation in the neutron-scattering experiments. We also find long-range Coulomb interaction to be less effective in the formation of half-doped stripes.

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The mechanism for the formation of the stripe states has been one of the most important issues in understanding high-temperature superconducting cuprates. Although many theoretical works based on the electronic model alone have succeeded in comprehending experimental results qualitatively,[1,2] there are many puzzles on the stripe formation in the underdoped cuprates $La_{2-x}Sr_xCuO_4$ (LSCO) and $La_{2-x}Ba_xCuO_4$ (LBCO) with 1/8 doping most stable.[3–7] For instance, the doping dependence of the incommensurate magnetic peaks associated with the stripe determined by neutron-scattering experiment on LSCO obeys the so-called Yamada plot[4] where it points to the existence of the half-doped stripe with average of 1/2 hole in one charge modulation period below 1/8 hole density. Furthermore, at 1/8 doping of LBCO, the local density of states still has a V shape and a node at low energy[8,9] even though the superconductivity is almost completely suppressed by the static stripe. Surprisingly, a recent scanning tunneling spectroscopy has observed cluster glasses with randomly oriented domains of stripelike patterns in two other families of $Ca_{2-x}Na_xCuO_2Cl_2$ and $Bi_2Sr_2Dy_{0.2}Ca_{0.8}Cu_2O_{8+\delta}$.[10] So far all these results are yet to be explained theoretically in a strongly correlated framework.

Many early theoretical works have found that stripe-ordered formation may be present in the extended *t*-*J* Hamiltonian.[11–14] In particular, using the density-matrix renormalization group (DMRG) in the standard *t*-*J* models, the mechanism of the half-doped stripe appears to have been understood by antiferromagnetic correlation across the hole[15] or optimum energy per hole of a domain wall.[16] However due to small lattice size, weak-coupling treatment, and special boundary conditions used in these works, this issue is still being debated.[17] The result of DMRG indicated the stripe to be most stable when the second nearest-neighbor hopping, t', is very small. This result is exactly opposite to the previous variational Monte Carlo (VMC) calculation.[13] Based upon the idea of *d*-wave resonating-valence-bond (*d*-RVB) state, recently we have proposed a stripe-ordered wave function which involves modulations of charge, spin magnetization, and pair field. These stripe states either in a periodic pattern or a randomly oriented domain have almost the same energy as the uniform *d*-RVB state for almost all values of t'/t in the extended *t*-*J* model.[18,19] This unexpected energy degeneracy of stripe-ordered states seems to be quite compatible with the proposal of fluctuating stripes.[20,21] However, this degeneracy between different stripe orders and a uniform state in the *t*-*J*-type model fails to explain the prominence of the half-doped stripes.

There are several possibilities for the formation of stripes. Long-range Coulomb interaction between holes has been proposed sometime ago to transform the frustrated phase separation into a stripe state.[22,23] On the other hand, a number of experiments have presented evidences that phonon or lattice effects are apparently present in these materials.[24–27] Particularly, due to the structural instability, the isotope effect in LSCO and LBCO is also peculiarly strong near 1/8 doping.[28] Moreover, to understand a kink structure in angle-resolved photoemission spectrum,[29] many theoretical works have accepted that the electron-phonon couplings should be considered in the *t*-*J*-type models.[30–35]

In this Rapid Communication, we shall consider both long-range Coulomb interaction and electron-phonon interaction on the formation of stripes, in particular half-doped stripes, within the context of strong correlation as in the extended *t*-*J* model. However electron-phonon interaction has many effects. We will only examine the simplest effect of mass renormalization of charges due to phonon coupling when the coupling strength is rather weak. The renormalization effect depending on the local charge density is treated self-consistently in a VMC method which takes into account the strong correlation accurately. In the latter half of the Rapid Communication, we present results of including long-ranged repulsive interaction between holes in the *t*-*J* Hamiltonian without electron-phonon interaction.

Let us begin with an extended *t*-*J* Hamiltonian in a two-dimensional square lattice which is defined as

$$H = -\sum_{i,j,\sigma} t_{ij}(\tilde{c}^{\dagger}_{i\sigma}\tilde{c}_{j\sigma} + \text{H.c.}) + J\sum_{\langle i,j\rangle} \mathbf{S}_i \cdot \mathbf{S}_j. \quad (1)$$

The hopping amplitude $t_{ij}=t$, t', and t'' for sites i and j being the nearest, second-nearest, and third-nearest neighbors, respectively. Other notations are standard. In the following, we focus on the case $(t',t'',J)/t=(-0.2,0.1,0.3)$ as we have shown[18] that comparing with the uniform state, energies of the stripe state are not very sensitive to the values of t'/J and

t''/J. Following our treatment in Ref. 18, the stripe wave function is constructed by the mean-field Bogoliubov–de Gennes method. We assume that the spatial dependence of the local charge density ρ_i, staggered magnetization m_i, and nearest-neighbor pair field Δ_{ij} has the simple forms:

$$\rho_i = \rho_v \cos[2q \cdot (y_i - y_0)],$$

$$m_i = m_v \sin[q \cdot (y_i - y_0)],$$

$$\Delta_{i,i+\hat{x}} = \Delta_v^M \cos[2q \cdot (y_i - y_0)] - \Delta_v^C,$$

$$\Delta_{i,i+\hat{y}} = -\Delta_v^M \cos[2q \cdot (y_i - y_0) + q] + \Delta_v^C, \quad (2)$$

where $q=2\pi/a_s$ and a_s is the period or magnetic period of the stripe which is twice the charge period. Here the stripe extends uniformly along $\hat{x}$ direction, and y_0 is 1/2 (0) for the bond-centered (site-centered) stripe. Site-centered stripe will not be considered throughout the Rapid Communication unless specifically mentioned. This state called antiferromagnetic RVB (AF-RVB) stripe state[18] is quite different from the antiphase stripe studied by others.[13] The magnitude of pair field and the magnetization are larger at sites with smaller hole density. Once the variational parameters are given, we diagonalize the mean-field Hamiltonian. Then, the trial wave function with a Gutzwiller projector P_G can be constructed by creating all negative energy states $\bar{\gamma}_n^\dagger$ and annihilating all positive energy states γ_n on a vacuum of electrons $|0\rangle$, $P_G P_J P_{N_e} \Pi_n \gamma_n \bar{\gamma}_n^\dagger |0\rangle$, with the fixed number of electrons N_e. Here we introduce a particle-hole transformation,[36] $c_{i\uparrow}^\dagger \rightarrow f_i$ and $c_{i\downarrow}^\dagger \rightarrow d_i^\dagger$. Using this transformation, we avoid the possibility of having a divergent determinant because of the presence of nodes in RVB-type wave function with the fixed number of particles using periodic boundary condition. We also introduce a hole-hole repulsive Jastrow factors P_J in order to greatly improve the variational energies (see the details in Ref. 18).

The simplest effect of an electron-phonon interaction is to renormalize the mass of charge carriers. To take into account of it within the extended t-J model, we assume the hopping terms t_{ij} in Eq. (1), which are inversely proportional to the effective mass, are modified due to the spatial variation in hole density. We neglect the renormalization of the exchange interaction J since it is only dominant in the very underdoped region with a very small effect.[31] We also do not consider the on-site energy that may arise from the electron-phonon coupling.[37] If the on-site energy varies linearly with the local hole density, it will have the same energy irrespective of the period of periodic stripes. According to the experimental results that the electron-phonon coupling strength λ is reduced by the hole density δ,[35] we assume a linear relation between λ and δ, $\lambda(\delta)/\lambda(0) \equiv f(\delta) = 1 - 3\delta$ (see the inset in Fig. 1). Accordingly, sites with a larger hole density in a modulated charge pattern have larger t_{ij}.[38] Thus t_{ij} in Eq. (1) is renormalized to t_{ij}^*, given by

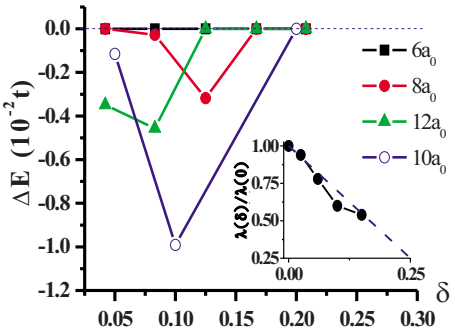

FIG. 1. (Color online) The optimized energy difference between the AF-RVB stripe and uniform d-RVB states vs the doping density δ for different periods of stripe. $10a_0$ is calculated in 20×20 lattice and others in 24×24 one. Here Λ is 0.25. Inset: the electron-phonon coupling constant vs hole density. Filled circles show the data points from Ref. 35. The dashed line is $1-3\delta$.

$$t_{ij}^* = t_{ij}\left\{1 - \Lambda\left[\frac{f(n_h^i) + f(n_h^j)}{2}\right]\right\}, \quad (3)$$

where n_h^i is the hole density at site i and $\Lambda = \lambda(0)/\pi$. We estimate a reasonable range of Λ should be from 0 to 0.25.[38] Since λ depends on the hole density n_h^i, we have to do a self-consistent calculation to find the minimal variational energy. Here we use the iterative method to achieve the convergence. First we assume an initial set of values for the hole density at different sites such that t_{ij}^* are given, then we can proceed to optimize the trial wave functions. If the hole densities calculated by this optimized wave function do not agree with the initial input values, we will then use the calculated density, hence its t_{ij}^*, as input value for the next round of optimization. This process is repeated until we have a converged result. Sometimes we also try to use either the overestimated or underestimated densities as initial input values to examine the convergence.

Figure 1 shows the energy gain per site obtained by the AF-RVB stripe states as a function of doping density in the $t-t'-t''-J$ model with renormalized t^*. The reference ground state is the uniform d-RVB wave function. Comparing to our previous work,[18] the hopping modulation due to electron-phonon coupling indeed stabilizes the AF-RVB stripe states in the underdoped regime ($\delta \sim 0.05-0.15$). The AF-RVB stripes with different periods of magnetic modulation such as $8a_0$, $10a_0$, and $12a_0$ have its minimum at doping density 1/8, 1/10, and 1/12, respectively, which is exactly half-doped with 1/2 hole per charge domain. We have not found a stable stripe with period $6a_0$. Above doping density greater than 1/8, none of the stripe states are particularly stable. These results are quite consistent with the "Yamada plot" observed in several experiments,[3,4,6] except that we have not studied the diagonal stripes below hole density of 0.05. Furthermore, to make sure $8a_0$ is indeed most stable at 1/8 doping, we also calculate the energy of a "one-doped stripe" with spin modulation $16a_0$ in a 16×16 lattice. The AF-RVB stripe with $16a_0$ is found to be energetically unstable with respect to $8a_0$.

At 1/8 doping, Fig. 2(a) shows that in contrast with $6a_0$

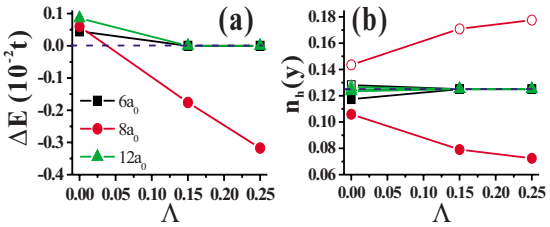

FIG. 2. (Color online) (a) The optimized energy difference between the AF-RVB stripe and uniform d-RVB states vs Λ. (b) The average hole density of the AF-RVB stripes with different magnetic periods vs Λ. For $6a_0$ and $8a_0$, empty (filled) symbols indicate $n_h(y=1)$ $[n_h(y=2)]$. As for $12a_0$, empty, half-filled, and filled symbols correspond to $n_h(y=1)$, $n_h(y=2)$, and $n_h(y=3)$, respectively. Here the doping is 1/8.

and $12a_0$, the energy gain of AF-RVB stripe state with $8a_0$ increases with the strength of Λ. As shown in Fig. 2(b), the difference in the average hole density between hole-rich and hole-poor domains becomes larger as Λ increases. Among all possible magnetic periods of stripes, only the stripe with $8a_0$ is stable at 1/8 doping. We also find that long-range pair-pair correlation function for the AF-RVB stripe states is reduced at 1/8 doping (not shown), which could explain the superconducting transition temperature is suppressed near 1/8 doping for LBCO.[39]

In order to understand the stability of half-doped stripe, we examine the spatial distribution of hole density $n_h(i)(=1-\tilde{c}^{\dagger}_{i\sigma}\tilde{c}_{i\sigma})$ as a function of doping density δ. In Fig. 3(a), the $8a_0$ stripe only has two distinct sites along $\hat{y}$ direction. When the difference of hole density between these two sites is getting larger, the state gains more kinetic energy from the modulated hopping terms as there are more holes sitting at sites with larger t^*. Interestingly, the maximum energy gain (see the filled circles in Fig. 1) with the largest difference in hole density exactly happens at 1/8 doping for $8a_0$ stripe. At doping density 1/6 or higher, the kinetic energy for the uniform state is already quite substantial, hence the separation of hole-rich sites and hole-poor sites does not gain enough energy and we do not find a stable periodic stripe with $8a_0$. This argument also holds for stripe with other periods so there is no stable periodic stripe state in optimum or overdoped systems. In the very underdoped regime, since the hole density is already small, separation into a hole-rich and a hole-poor site does not bring a large difference to gain enough kinetic energy to stabilize the periodic stripes. However, for stripes with $10a_0$ and $12a_0$ shown in Fig. 3(b), there are three different sites with only one of them having more hole density than the uniform state. There is again the maximum difference in hole density occurs at smaller dopings (1/10 and 1/12, respectively). Similar argument also holds for $10a_0$ and $12a_0$ stripes.

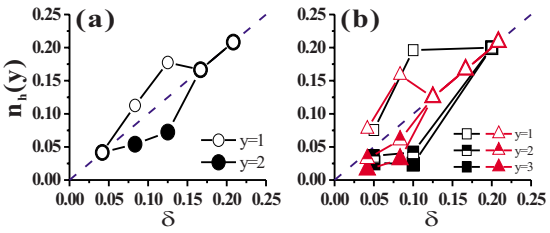

FIG. 3. (Color online) The average hole density of the AF-RVB stripes with the (a) $8a_0$, (b) $10a_0$ (squares), and $12a_0$ (triangles) vs the doping density δ using the same parameters in Fig. 1. Different symbols denote different average hole densities along $\hat{y}$ direction. The dashed line is the doping density.

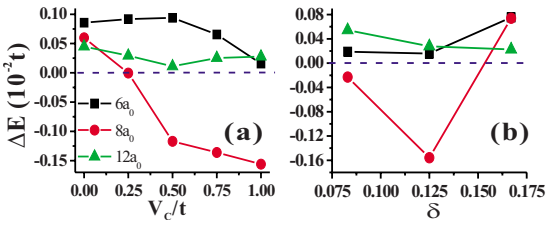

FIG. 4. (Color online) (a) The optimized energy difference between the AF-RVB stripe and uniform d-RVB states as a function of the strength of Coulomb interaction V_C at 1/8 doping. (b) The optimized energy difference vs doping density δ for $V_C/t=1$.

The argument provided above for the stability of half-doped stripes could be applicable to other kinds of stripes. Hence we also examine the site-centered AF-RVB stripes and antiphase stripes at 1/8 doping. As expected, the site-centered stripes have similar results as bond-centered stripes discussed above except with higher per-site energy $(0.0022t)$ at $8a_0$. Similarly for the antiphase stripes $8a_0$ has lowest energy at 1/8 doping but it again has a slightly higher per-site energy $(0.0008t)$.

Finally, we investigate the stability of the AF-RVB stripes in $t-t'-t''-J$ system with long-range Coulomb interaction. In this case, the calculations omit the mass renormalization in the Hamiltonian for the moment. The Coulomb interaction between holes is given by $V_C\Sigma_{i<j}n_h(i)n_h(j)/|\mathbf{r}_i-\mathbf{r}_j|$. We have only studied stripes with periods $6a_0$, $8a_0$, and $12a_0$. The modulation of hole density and staggered magnetization is enhanced by Coulomb interaction. In Fig. 4(a), as V_C increases, only the $8a_0$ stripe pattern becomes more stable which is consistent with previous DMRG studies.[12] As shown in Fig. 4(b), the $6a_0$ and $12a_0$ stripes always have higher energy than uniform d-RVB state even for $V_C=t$. Although the stripe with $8a_0$ is stabilized at 1/8 doping, its energy gain is about half of that obtained by the mass renormalization effect shown in Fig. 2(a). These results indicate that although the long-range Coulomb interaction could help the formation of stripes, it is not particularly effective in getting the half-doped stripes as the electron-phonon coupling.

To summarize, we have successfully included the effect of mass renormalization due to weak electron-phonon interaction with the extended t-J Hamiltonian in a self-consistent VMC calculation. It is shown that the vertical half-doped stripes are most preferred in the underdoped regime with hole density $1/12 \leq \delta \leq 1/8$. This explains the Yamada plot mostly seen in LSCO materials. Since the stability of stripes is enhanced by electron-phonon coupling, our result also implies that this coupling is stronger in LSCO materials than other cuprates which is consistent with the analysis of kink in Ref. 29. Additionally, we have found that long-range Coulomb interaction does not play as an important role in the formation of half-doped stripes as the mass renormalization effect due to electron-phonon interaction.

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