PHYSICAL REVIEW B, VOLUME 63, 140509(R)

Stripes due to the next-nearest-neighbor exchange in high-T_c cuprates

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(Received 2 January 2001; published 22 March 2001)

We propose a possible mechanism of the charge stripe order due to the next-nearest-neighbor exchange interaction J' in the two-dimensional t-J model, based on the concept of the phase separation. We also calculate some hole correlation functions of the finite cluster of the model using the numerical diagonalization, to examine the realization of the mechanism. It is also found that the next-nearest-neighbor hopping t' suppresses the stripe order induced by the present mechanism for $t'<0$, while it enhances for $t'>0$.

DOI: 10.1103/PhysRevB.63.140509 PACS number(s): 74.72.Dn, 71.10.Fd, 71.45.Lr

The charge stripe order[1,2] observed in the high-temperature cuprates superconductors is one of the most interesting current topics on the strongly correlated electron systems. In particular, since the discovery of the coexistence with the superconductivity in $La_{1.6-x}Nd_{0.4}Sr_xCuO_4$,[3] the mechanism of the stripe formation has been studied in many works. The numerical study[4] based on the density matrix renormalization group suggesting that such a stripe phase can appear in the two-dimensional t-J model. On the other hand, the numerical diagonalization of the 4×4 t-J cluster with two holes[5] indicated that the stripe order occurs only in some low-lying excited states, rather than the ground state. The realization of the stripe order in the simple t-J model is still an open problem.

It is well known that the t-J model should exhibit the phase separation for sufficiently large J/t.[6] The high temperature expansion suggested such a state is realized for $J/t\geqslant 1$.[7] Some small cluster calculations have shown that a larger cluster of holes is stable, rather than a pair, even in a more realistic parameter region ($J/t\geqslant 0.5$).[8] In the present paper, we propose a possible mechanism of the stripe order formation due to the additional next-nearest-neighbor exchange interaction J' based on a naive argument valid in the phase separation region of the t-J model. Since the next-nearest-neighbor hopping t' has been revealed to be quite large for $Sr_2CuO_2Cl_2$ ($t'\sim 0.3t$),[9] J' is also expected to be finite in some real cuprates. Thus we consider the square-lattice t-t'-J-J' model, and discuss the mechanism of the stripe as it relates to this model. We also calculate the three- and four-hole correlation functions of the 4×4 cluster with four holes, to examine the realization of the mechanism.

We consider the two-dimensional t-J model in the presence of the next-nearest-neighbor hopping t' and the exchange interaction J'. The Hamiltonian is given by the form

$$H=-t\sum_{\langle \mathbf{i},\mathbf{j}\rangle,\sigma}(c^\dagger_{\mathbf{j},\sigma}c_{\mathbf{i},\sigma}+c^\dagger_{\mathbf{i},\sigma}c_{\mathbf{j},\sigma})-t'\sum_{\langle \mathbf{i},\mathbf{j}\rangle',\sigma}(c^\dagger_{\mathbf{j},\sigma}c_{\mathbf{i},\sigma}+c^\dagger_{\mathbf{i},\sigma}c_{\mathbf{j},\sigma})+J\sum_{\langle \mathbf{i},\mathbf{j}\rangle}\left(\mathbf{S_i}\cdot\mathbf{S_j}-\frac{1}{4}n_\mathbf{i}n_\mathbf{j}\right)+J'\sum_{\langle \mathbf{i},\mathbf{j}\rangle'}\left(\mathbf{S_i}\cdot\mathbf{S_j}-\frac{1}{4}n_\mathbf{i}n_\mathbf{j}\right), \tag{1}$$

where $\Sigma_{\langle \mathbf{i},\mathbf{j}\rangle}$ and $\Sigma_{\langle \mathbf{i},\mathbf{j}\rangle'}$ mean the summation over all the nearest-neighbor and the next-nearest-neighbor sites, respectively. Throughout the paper, all the energies are measured in units of t. We assume the next-nearest-neighbor exchange interaction is antiferromagnetic ($J'>0$), as was revealed for La_2CuO_4 by the theoretical study based on the *ab initio* calculation.[10] The antiferromagnetic J' term can also be derived from the strong correlation expansion of the Hubbard Hamiltonian up to the order of t^4/U^3.[11] Since t' plays no essential roles in the following argument, we set $t'=0$ first.

Consider the naive argument to explain the hole pairing due to the antiferromagnetic short range order: a pair of holes sitting on the adjacent cites is more stable than two separated holes, because the former breaks 7 J bonds, while the latter breaks 8 J bonds. Following the argument, larger hole clusters are expected to be formed for sufficiently large J. In such a situation we consider the effect of J'. (We assume J' is not so large that the antiferromagnetic short range order is completely broken.) At first we compare the stability of three-hole cluster in two different shapes, shown in Figs. 1(a) and 1(b), respectively. The number of J bonds are the same between them, but (a) has one more broken J' bond than (b). When the antiferromagnetic short range correlation is developed, the J bond should lead to the advantage of the energy, while the J' to the disadvantage, as far as J and J' are antiferromagnetic. Then (a) is expected to be more stable

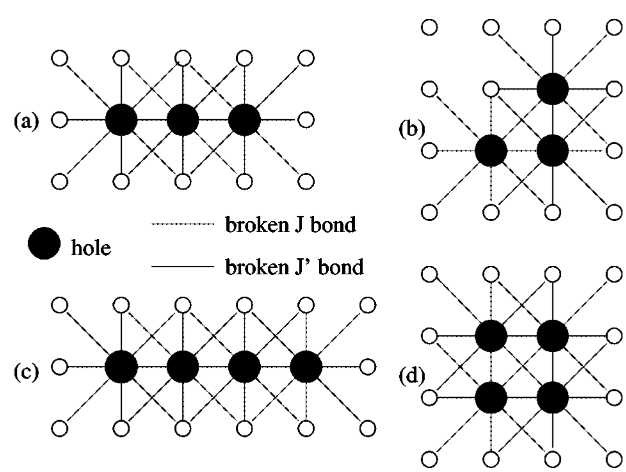

FIG. 1. Schematic figures to show on the stability of the three-hole and four-hole clusters.

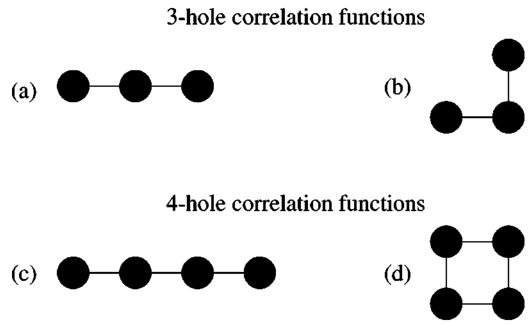

FIG. 2. Configurations of the many-hole correlation functions; (a) $C_{\rm St}^{(3)}$, (b) $C_{\rm PS}^{(3)}$, (c) $C_{\rm St}^{(4)}$, and (d) $C_{\rm PS}^{(4)}$.

than (b). Thus the three hole cluster should prefer the line shape shown in (a) to the corner shape shown in (b). Next we consider the four-hole cluster with the two shapes, shown in Figs. 1(c) and 1(d), respectively. In this case the number of J bonds is also different. One more J bond and two more J' bonds are broken in shape (c) as compared to (d). Assuming that the antiferromagnetic short range order is so large that the next-nearest-neighbor spin correlation is almost the same as the next one in amplitude, line shape (c) is more preferable than (d) under the condition $J' \geqslant J/2$. This condition is easily revealed to be approximately valid in comparison between the line-shaped and the square-shaped larger clusters with the same number of holes. Thus large line-shaped clusters of holes should be formed for sufficiently large J'. This naive argument is expected to provide a possible mechanism of the charge stripe order.

In order to examine the realization of the mechanism of the charge stripe order discussed in the previous section, we calculate the three- and four-hole correlation functions defined as

$$C_{\rm St}^{(3)} = \left\langle \sum_{\mathbf{i}} n_{\mathbf{i}}^h n_{\mathbf{i}+\hat{x}}^h n_{\mathbf{i}+2\hat{x}}^h \right\rangle, \tag{2}$$

$$C_{\rm PS}^{(3)} = \left\langle \sum_{\mathbf{i}} n_{\mathbf{i}}^h n_{\mathbf{i}+\hat{x}}^h n_{\mathbf{i}+\hat{x}+\hat{y}}^h \right\rangle, \tag{3}$$

$$C_{\rm St}^{(4)} = \left\langle \sum_{\mathbf{i}} n_{\mathbf{i}}^h n_{\mathbf{i}+\hat{x}}^h n_{\mathbf{i}+2\hat{x}}^h n_{\mathbf{i}+3\hat{x}}^h \right\rangle, \tag{4}$$

$$C_{\rm PS}^{(4)} = \left\langle \sum_{\mathbf{i}} n_{\mathbf{i}}^h n_{\mathbf{i}+\hat{x}}^h n_{\mathbf{i}+\hat{y}}^h n_{\mathbf{i}+\hat{x}+\hat{y}}^h \right\rangle, \tag{5}$$

in the ground state of the finite cluster t-t'-J-J' model ($t' = 0$). $C_{\rm St}^{(3)}$ and $C_{\rm St}^{(4)}$ are supposed to represent a relative strength of the stripe order, while $C_{\rm PS}^{(3)}$ and $C_{\rm PS}^{(4)}$ measure a tendency towards the ordinary phase separation. They are calculated for the 4×4 cluster with four holes, for which the ground state has the d-wave-like rotational symmetry for $J \geqslant 0.3$.[8] (See Fig. 2.) (We neglect the other ground states which appear in smaller J regions for simplicity.) The calculated three- and four-hole correlation functions are plotted versus J' with fixed J (=0.6 and 0.8), in Figs. 3 and 4, respectively. We detected a first-order transition (a level

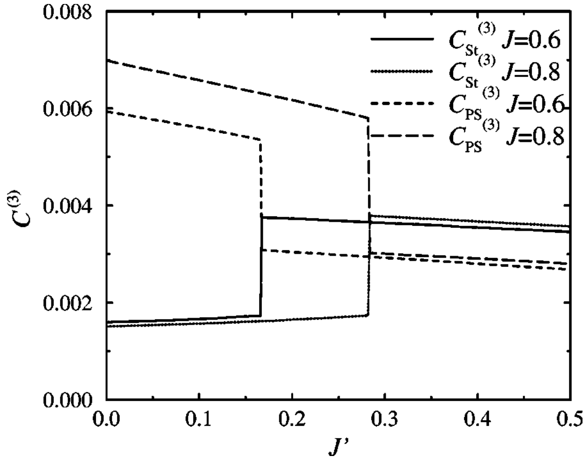

FIG. 3. Three-hole correlation functions versus J' with fixed J (=0.6 and 0.8).

cross) at some critical value J_c' (J_c' depends on J) and found that the line-shaped correlation is larger than the square-shaped one for $J' \geqslant J_c'$, while it is reversed for $J' \leqslant J_c'$ in both Figs. 3 and 4. This implies that the charge stripe order is possibly realized in the bulk system for sufficiently large J', in agreement with the mechanism proposed in the previous section. Then J_c' is expected to be the boundary between the phase separation and the stripe ordered phases in the thermodynamic limit. Plotting the calculated J_c' for various values of J, we give a phase diagram in the J'-J plane for $t'=0$ (solid circles) in Fig. 5. We can also understand that the excited state with the stripe order, which was found in the previous numerical study,[5] is stabilized by the next-nearest-neighbor exchange interaction in the upper phase in Fig. 5.

The phase diagram for $t'=0$ in Fig. 5 indicates an interesting point: the stripe order is possibly realized even if J' is much smaller than $J/2$ in the small-J region around $J \sim 0.4$, which is realistic for the high-T_c cuprates. Some recent theoretical analyses[12–14] on the simple t-J model actually revealed that the phase separation occurs even in such a realistic parameter region. The present result of the phase

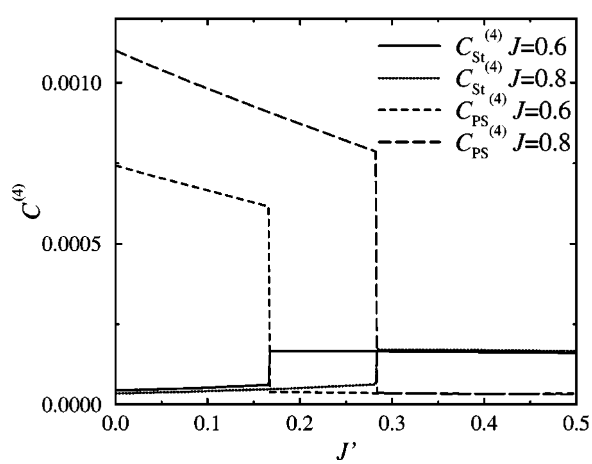

FIG. 4. Four-hole correlation functions versus J' with fixed J (=0.6 and 0.8).

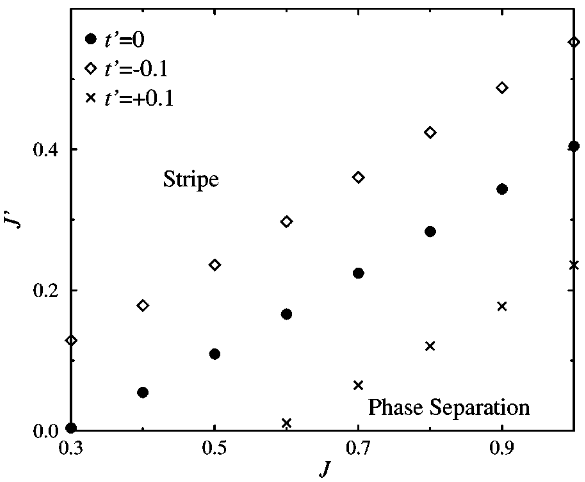

FIG. 5. Phase diagrams in the J'-J plane for $t'=0$, -0.1, and 0.1.

separation-stripe boundary $J_c \sim 0.3$ for $J'=t'=0$ in Fig. 5 is consistent with these results. It implies that the scenario of the stripe formation based on the next-nearest-neighbor exchange interaction is possibly valid for real cuprates, although the precise phase boundary is still controversial. Note that the present analysis does not distinguish between the static stripe order and the dynamical one, like the charge strings, which was predicted by the phonon-induced polaron mechanism.[15] It would be interesting to study such a dynamical stripe, which may provide some hints in explaining the coexistence of the stripe order and the superconductivity observed in $La_{1.6-x}Nd_{0.4}Sr_xCuO_4$.

Finally, we consider the effect of the next-nearest-neighbor hopping t' in the present mechanism of the stripe formation. For this purpose, the phase boundaries between the stripe and the pairing (or phase separation) phases for $t'=-0.1$ (diamonds) and $t'=0.1$ (crosses) are shown in Fig. 5. The negative and positive t' are corresponding to hole and electron doping cases, respectively. The phase diagram suggests that the negative t' suppresses the stripes, while the positive t' enhances it. The result agrees with the numerical studies,[16,17] at least for small t', although they did not consider J'. Our result implies that the stripe due to J' in the present mechanism has the same feature as the one which was investigated in those previous works. Actually, Fig. 5 indicates that the stripe can occur even for $J'=0$, at least in the case of the positive t'. It would be more interesting to perform the same calculation for a more realistic hole density, close to 1/8, if possible. (For example, the 32-site cluster with 4 holes is desirable, but it is difficult for the present computer systems.)

The recent high-resolution inelastic neutron scattering experiment[11] indicated that the ring (four-spin) exchange interaction is more important in explaining the observed spin-wave dispersion of La_2CuO_4, rather than the next-nearest-neighbor exchange interation. Thus we should also take the ring exchange interaction into account for a more quantitative study.

In summary, we proposed a possible mechanism of the charge stripe formation based on the next-nearest-neighbor exchange interaction J' in the high-T_c cuprates. The many-hole correlation functions of the 4×4 lattice t-t'-J-J' model indicated that even small J' possibly induces the stripe order for realistic values of J. In addition, the next-nearest-neighbor hopping t' was revealed to suppress the stripe for $t'<0$, but enhance it for $t'>0$.

We thank D. Poilblanc and T. M. Rice for fruitful discussions. The computation in this work has been done using the facilities of the Supercomputer Center, Institute for Solid State Physics, University of Tokyo. This research was supported in part by a Grant-in-Aid for the Scientific Research Fund from the Ministry of Education, Science, Sports and Culture (11440103).

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