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Investigation of charge stripe formation in an extended *t–J* model

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Abstract

We consider a possible mechanism of the charge stripes in the high-T_c cuprates, based on some additional interactions in the two-dimensional t–J model; the next-nearest-neighbour and/or four-spin (ring) exchange interactions. The many-hole correlation functions obtained by numerical exact diagonalization of a finite-cluster t–J model including the correction terms indicate the realization of the mechanism and give some preliminary phase diagrams. A realistic combination of these additional terms is also studied.

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1. Introduction

The charge stripe has attracted a lot of interest in the field of the strongly correlated electron systems. The charge stripe order in the high-T_c cuprates was observed by neutron scattering [1, 2] and x-ray absorption [3] etc. In order to explain the mechanism of the stripe formation, many theoretical mechanisms have been proposed based on some long-range Coulomb interactions or lattice distortions [4] etc. The realization of the stripe was discussed even in the framework of the simple t–J model [5, 6]. The real mechanism, however, is still an open problem. Recently, the coexistence of the stripe and the superconductivity was observed in $La_{1.6-x}Nd_{0.4}Sr_xCuO_4$ [7]. This indicates that the mechanism of the stripe is not based only on the static lattice distortion which should lead to a localization due to a polaron effect.

In the previous work [8], the present author indicated that the next-nearest-neighbour exchange interaction can be one of the origins of the charge stripe, based on the short-range antiferromagnetic correlation leading to the phase separation. On the other hand, the recent neutron scattering measurement [9] on La_2CuO_4 revealed that the four-spin cyclic (ring)

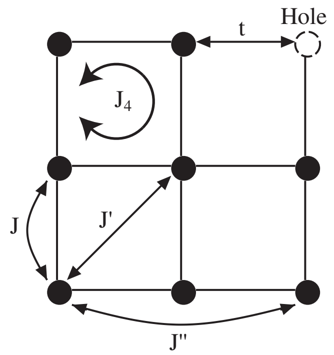

Figure 1. Schematic figure of the extended t–J model, including the second- and third-neighbour exchange interactions, as well as the four-spin cyclic exchange.

exchange interaction at each plaquette is more significant than the next-nearest-neighbour two-spin exchange. The previous numerical study of a finite-cluster extended t–J model suggested that the four-spin exchange stabilizes the stripe formation caused by the next-nearest-neighbour two-spin exchange interaction [10]. In the present paper, we explain that the ring exchange is possibly an important origin of the charge stripe more explicitly, based on a naive argument of the frustration and the numerical diagonalization study. We also investigate a realistic combination of the two- and four-spin exchange interactions, and present a preliminary phase diagram of an extended t–J model on the square lattice obtained by a finite-cluster calculation.

2. Extended *t*–*J* model

In order to investigate the mechanism of the charge stripe formation based on the next-nearest-neighbour and/or four-spin exchange interaction, we consider the two-dimensional extended t–J Hamiltonian as follows:

$$H = -t \sum_{\langle \mathbf{i},\mathbf{j}\rangle,\sigma} \left(c^{\dagger}_{\mathbf{j},\sigma} c_{\mathbf{i},\sigma} + c^{\dagger}_{\mathbf{i},\sigma} c_{\mathbf{j},\sigma}\right) + J \sum_{\langle \mathbf{i},\mathbf{j}\rangle} \left(\mathbf{S_i}\cdot\mathbf{S_j} - \frac{1}{4} n_{\mathbf{i}} n_{\mathbf{j}}\right) + J' \sum_{\langle \mathbf{i},\mathbf{j}\rangle'} \left(\mathbf{S_i}\cdot\mathbf{S_j} - \frac{1}{4} n_{\mathbf{i}} n_{\mathbf{j}}\right)$$
$$+ J'' \sum_{\langle \mathbf{i},\mathbf{j}\rangle''} \left(\mathbf{S_i}\cdot\mathbf{S_j} - \frac{1}{4} n_{\mathbf{i}} n_{\mathbf{j}}\right) + J_4 \sum_{\mathbf{j}} \left(P_{4,\mathbf{j}} + P^{-1}_{4,\mathbf{j}}\right) \tag{1}$$

where $\sum_{\langle \mathbf{i},\mathbf{j}\rangle}$, $\sum_{\langle \mathbf{i},\mathbf{j}\rangle'}$ and $\sum_{\langle \mathbf{i},\mathbf{j}\rangle''}$ are the sums over the first-, second- and third-neighbour bonds, respectively. We also put the third-neighbour exchange interaction J'', because it is of the same order as J' and J_4 in the perturbation expansion from the large-U limit of the Hubbard Hamiltonian [11]. $P_{4,\mathbf{j}}$ is the cyclic permutation operator which exchanges the four spins around the $\mathbf{j}$th plaquette as $\mathbf{S_j} \rightarrow \mathbf{S}_{\mathbf{j}+\hat{x}} \rightarrow \mathbf{S}_{\mathbf{j}+\hat{x}+\hat{y}} \rightarrow \mathbf{S}_{\mathbf{j}+\hat{y}} \rightarrow \mathbf{S_j}$, J_4 is the strength of the four-spin ring exchange. Although the long-range hopping terms t' and t'' are also known to exist in real cuprates, we neglect them because they play no essential role for the present mechanism. We assume all the two-spin exchange interactions are antiferromagnetic, namely J, J' and J'' are positive. The schematic figure of the model is shown in figure 1. Throughout the paper, all the energies are measured in units of t.

3. Mechanism of charge stripe formation

3.1. Next-nearest-neighbour exchange

At first we review the mechanism of the charge stripe due to the next-nearest-neighbour exchange interaction, discussed in [8]. According to the well-known naive argument on the hole pairing in the *t–J* model, two holes in the background of the short-range antiferromagnetic order for sufficiently large J/t tend to form the nearest-neighbour pair. This is because the pair breaks seven J bonds, while two separate holes break eight, so the pair is more stable by the energy of a J bond. The argument leads to phase separation in many hole systems. Indeed, the *t–J* model was revealed to exhibit phase separation for sufficiently large J/t [12]. The high temperature expansion suggested that such a state is realized for $J/t \geqslant 1$ [13]. Some small cluster calculations have shown that a larger cluster of the holes is stable rather than a pair, even in a more realistic parameter region ($J/t \geqslant 0.5$) [14]. Some recent theoretical analyses [15–17] on the simple *t–J* model actually revealed that the phase separation occurs even in a parameter region $J/t = 0.2$–0.4, realistic for the cuprates. Thus, we assume phase separation is realized.

We assume the next-nearest-neighbour exchange interaction is antiferromagnetic, as was revealed for La_2CuO_4 by the theoretical study based on the *ab initio* calculation [18]. Applying a similar argument for the *t–J* model including J', the system is more stable when more J' bonds are broken, because the antiferromagnetic J' is frustrated with the short-range order due to J. In order to consider the stability of the vertical (or horizontal) charge stripe, we compare the two shapes of hole clusters; (a) square and (b) line, which mean ordinary phase separation and the stripe, respectively. They are shown in figures 2(*a*) and (*b*), respectively. In figures 2(*a*) and (*b*), solid and open circles denote electrons and holes, respectively. Solid lines (with arrows) denote J (J') bonds, and dashed lines mean broken bonds. If we neglect the surface region of the clusters, the *N*-hole square cluster breaks $\sim 2N\ J$ and $\sim 2N\ J'$ bonds, while the *N*-hole line cluster breaks $\sim 3N\ J$ and $\sim 4N\ J'$ bonds. Thus, the short-range antiferromagnetic correlation would stabilize the line cluster $(2J' - J)N$ more. Therefore, the line hole cluster is possibly more preferable than the square for sufficiently large J' ($J' > J/2$). This is why the next-nearest-neighbour exchange interaction is a possible driving force of the charge stripes.

3.2. Ring exchange

The recent neutron scattering measurement [9] suggested that the ring exchange interaction J_4 is more important than J'. In fact, the perturbation expansion of the Hubbard Hamiltonian [11] from the large-U limit gave the parameters of the extended *t–J* model (1) as follows:

$$J' = J'' = \frac{J_4}{20} = \frac{4t^4}{U^3}. \tag{2}$$

It was also justified by the neutron scattering experiment. If the form (2) is assumed, the measured dispersion is well explained with $J_4 \sim 0.3J$. In addition, the numerical diagonalization study on finite Heisenberg clusters [19] indicated that the ring exchange is important to explain the Raman scattering experiment on the undoped cuprate [20]. Thus, we consider the effect of J_4 in the presence of short-range antiferromagnetic order.

Based on a similar argument to J', we will also show that the ring exchange J_4 possibly leads to the charge stripe in the following. Note that a realistic J_4 is positive, which was justified by the above perturbative expansion from the Hubbard Hamiltonian and the neutron scattering experiment. If we consider only a single plaquette with four spins, the

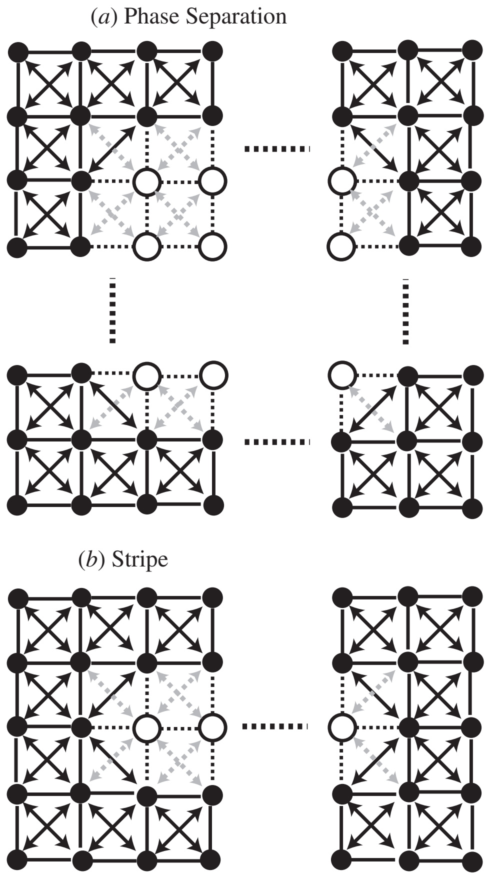

Figure 2. (a) Square and (b) line hole clusters imply phase separation and the charge stripe, respectively. Solid and open circles denote electrons and holes, respectively. Solid lines (with arrows) denote active J (J') bonds, and dashed lines mean broken bonds.

nearest-neighbour exchange interaction J leads to the singlet ground state, while positive J_4 stabilizes the triplet state. Thus, it is expected that J_4 yields a kind of frustration with the original short-range antiferromagnetic correlation due to J. It implies that more broken plaquettes, where J_4 does not work, should have an advantage in energy for sufficiently large J/t and J_4/t. We consider the two shapes of hole clusters in figures 3(a) and (b), and discuss J'. In the figures, arcs with arrows indicate active ring exchange interactions and blank plaquettes mean broken ones. If we neglect the surface, the number of broken plaquettes is $\sim N$ for the square cluster, while $\sim 2N$ for the line. Thus, the line cluster should be more stable than the square one for sufficiently large J_4. Therefore, ring exchange is also a possible origin of the charge stripes.

4. Exact diagonalization study

In the previous section, the effect of the hole hopping term t is neglected. In order to confirm the above mechanisms of the stripe for finite t, we performed a numerical diagonalization

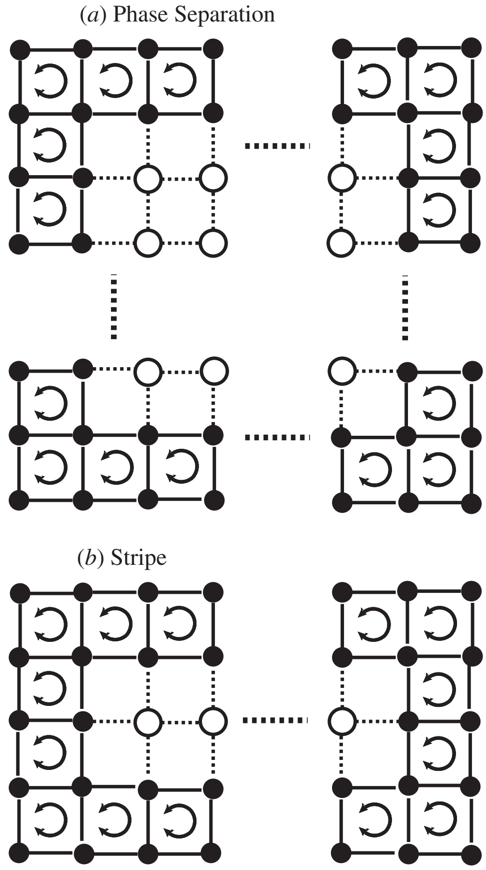

Figure 3. (*a*) Square and (*b*) line hole clusters imply phase separation and the charge stripe, respectively. Solid and open circles denote electrons and holes, respectively. Solid lines denote active J bonds, and dashed lines mean broken bonds. Arcs with arrows indicate active ring exchange interactions and blank plaquettes mean broken ones.

study with the Lanczos algorithm on the extended t–J model (1) on the 4×4 cluster with four holes under the periodic boundary condition.

In order to compare the two shapes of the hole cluster (line and square) in stability, we calculate the four-hole correlation functions defined as

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

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

in the ground state of the finite cluster extended t–J model (1). Their configurations are shown schematically in figures 4(*a*) and (*b*), respectively. $C_{\mathrm{PS}}^{(4)}$ measures a tendency towards ordinary phase separation, while $C_{\mathrm{St}}^{(4)}$ represents the relative strength of the stripe order.

At first, we put $J'' = J_4 = 0$ to clarify the stripe formation due to the next-nearest-neighbour exchange J', as studied in the previous work [8]. The calculated four-hole correlation functions are plotted versus J' with fixed J (=0.6) in figure 5. We detected a

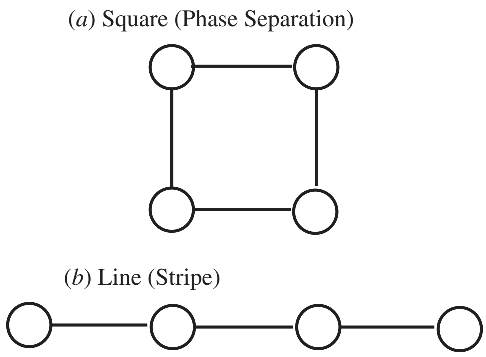

Figure 4. Schematic figures of two types of four-hole correlation functions; (*a*) square and (*b*) line shape, denoted as $C^{(4)}_{\mathrm{PS}}$ and $C^{(4)}_{\mathrm{St}}$.

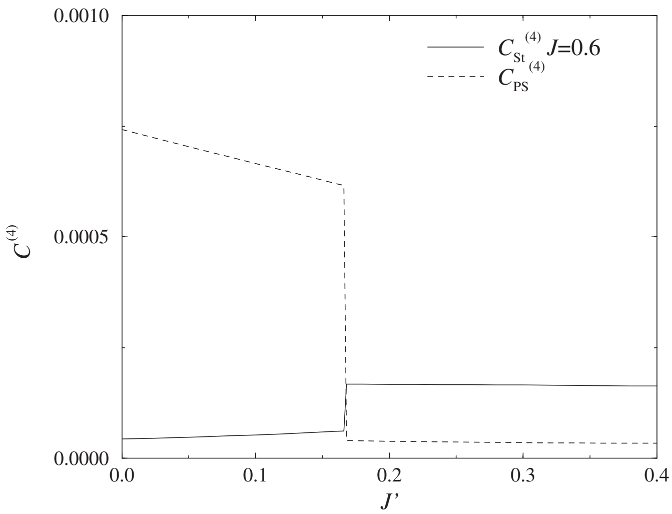

Figure 5. Four-hole correlation functions versus J' for fixed $J = 0.6$.

first-order transition (a level cross) at some critical value J'_c 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 figure 5. It 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 $J_4 = 0$ (a solid line) in figure 6.

Next we investigate the effect of the ring exchange interaction J_4 on the J'–J phase boundary. The same phase boundaries are shown for $J_4 = +0.1$ and -0.1, which are dotted and dashed lines, respectively, in figure 6. The realistic positive J_4 is revealed to shift down the phase boundary, while the negative J_4 shifts it up. It implies that the real ring exchange stabilizes the stripe phase due to J'. The behaviour of the phase boundary on the $J' = 0$ axis indicates that even only J_4 possibly realizes the same stripe phase.

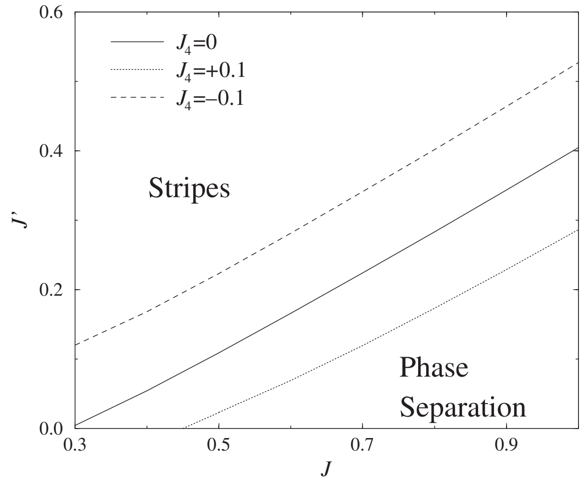

Figure 6. Phase diagrams in the J'–J plane for $J_4 = 0$, +0.1 and -0.1.

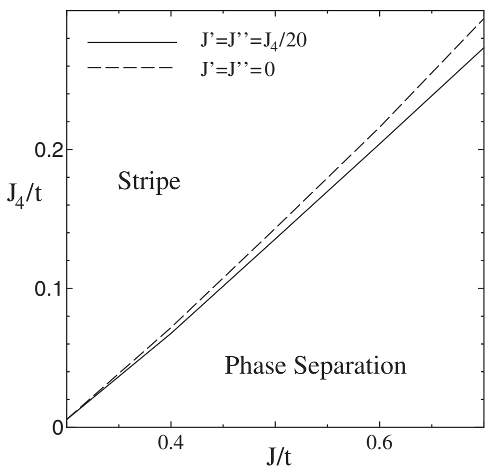

Figure 7. Phase diagrams in the J_4–J plane for $J' = J'' = 0$ and $J' = J'' = J_4/20$.

Finally, we show the J_4–J phase diagram in figure 7, based on the same calculation. The dashed line for $J' = J'' = 0$ indicates that only even J_4 leads to the same stripe phase as the one casued by J'. The solid line is the phase boundary for the most realistic combination of J', J'' and J_4, determined by the form (2) based on the strong correlation expansion from the Hubbard model and consistent with the neutron scattering experiment. The realistic parameter region $J/t = 0.3$–0.4 and $J_4 \sim 0.3J$ for the real cuprates is in the stripe phase in figure 7. Although the hole density of the present calculation (1/4) is far from the optimum one for the observed charge stripes (1/8), the essential point of the present mechanism is independent of the density. Thus, the second-, third-neighbour and ring exchange interactions should be a possible origin of the real charge stripes in the cuprates. We hope some larger-cluster calculation will be performed to approach the optimum density 1/8 in the near future.

The present analysis does not distinguish between the static stripe order and the dynamical one like the charge strings [21]. It would also be interesting to study such a dynamical stripe, which may provide some hints in explaining the coexistence of the stripe and superconductivity.

5. Summary

The numerical study on the extended t–J model indicated that the four-spin ring exchange interaction and/or the next-nearest-neighbour exchange interaction are possibly one of the origins of the charge stripe in the high-T_c cuprates.

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