Vol. 34 (2003) *ACTA PHYSICA POLONICA B* No 2

CHARGE STRIPES AND FOUR-SPIN EXCHANGE INTERACTION IN HIGH-T_c CUPRATES*

Tôru Sakai

Department of Physics, Tohoku University
Aramaki, Aoba-ku, Sendai 980-8578, Japan

(Received July 10, 2002)

A possible mechanism of the charge stripe due to the four-spin cyclic exchange interaction in the high-T_c cuprate is proposed. The realization of the mechanism is demonstrated by the numerical diagonalization of an extended t–J model.

PACS numbers: 74.72.Dn, 71.10.Fd, 71.45.Lr

The charge stripe is one of interesting topics in the field of the strongly correlated electron systems. Since the stripe order was observed in the high-T_c cuprate superconductors [1], many theoretical mechanisms have been proposed based on some long-range Coulomb interactions or lattice distortions *etc.* The realization of the stripe was discussed even in the framework of the simple t–J model. [2] The real mechanism, however, is still an open problem. In the previous work [3] the present author indicated that the 2nd neighbor exchange interaction can be one of the origins of the charge stripe. On the other hand, the recent neutron scattering measurement [4] on La_2CuO_4 revealed that the four-spin cyclic exchange interaction at each plaquette is more significant than the 2nd-neighbor two-spin exchange. In the present paper, we suggest that the four-spin exchange possibly leads to the charge stripe, as well as the 2nd-neighbor one, and present a preliminary phase diagram of an extended t–J model on the square lattice obtained by a finite-cluster calculation.

In order to investigate on the four-spin exchange as a driving force of the charge stripe, we consider the 2D extended t–J Hamiltonian as follows:

* Presented at the International Conference on Strongly Correlated Electron Systems, (SCES 02), Cracow, Poland, July 10–13, 2002.

$$
\begin{aligned}
H \;=\; & -t \sum_{\langle \boldsymbol{i},\boldsymbol{j}\rangle,\sigma} (c^{\dagger}_{\boldsymbol{j},\sigma} c_{\boldsymbol{i},\sigma} + c^{\dagger}_{\boldsymbol{i},\sigma} c_{\boldsymbol{j},\sigma}) + J \sum_{\langle \boldsymbol{i},\boldsymbol{j}\rangle} (\boldsymbol{S_i}\cdot\boldsymbol{S_j} - \tfrac{1}{4} n_{\boldsymbol{i}} n_{\boldsymbol{j}}) \\
& + J' \sum_{\langle \boldsymbol{i},\boldsymbol{j}\rangle'} (\boldsymbol{S_i}\cdot\boldsymbol{S_j} - \tfrac{1}{4} n_{\boldsymbol{i}} n_{\boldsymbol{j}}) + J'' \textstyle\sum_{\langle \boldsymbol{i},\boldsymbol{j}\rangle''} (\boldsymbol{S_i}\cdot\boldsymbol{S_j} - \tfrac{1}{4} n_{\boldsymbol{i}} n_{\boldsymbol{j}}) \\
& + J_4 \sum_{\boldsymbol{j}} (P_{4,\boldsymbol{j}} + P^{-1}_{4,\boldsymbol{j}}) \,, \qquad (1)
\end{aligned}
$$

where $\sum_{\langle \boldsymbol{i},\boldsymbol{j}\rangle}$, $\sum_{\langle \boldsymbol{i},\boldsymbol{j}\rangle'}$ and $\sum_{\langle \boldsymbol{i},\boldsymbol{j}\rangle''}$ are the sums over the 1st, 2nd and 3rd neighbor bonds, respectively. $P_{4,\boldsymbol{j}}$ is the cyclic permutation operator which exchanges the four spins around the $\boldsymbol{j}$-th plaquette as $\boldsymbol{S_j} \to \boldsymbol{S}_{\boldsymbol{j}+\hat{x}} \to \boldsymbol{S}_{\boldsymbol{j}+\hat{x}+\hat{y}} \to \boldsymbol{S}_{\boldsymbol{j}+\hat{y}} \to \boldsymbol{S_j}$, 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 Fig. 1.

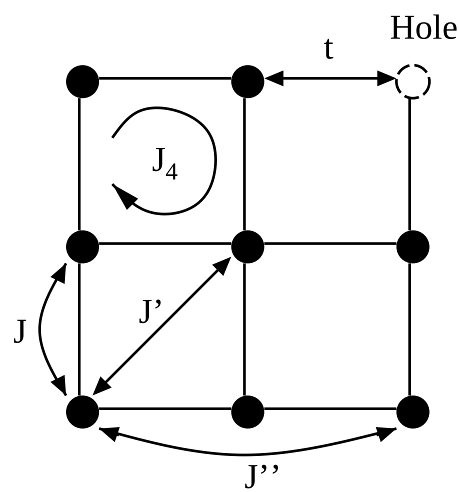

Fig. 1. Schematic figure of the extended t–J model, including the second and third neighbor exchange interactions, as well as the four spin cyclic exchange.

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-neighbor pair. This is because the pair breaks seven J bonds, while two separate holes breaks eight, so the pair is more stable by the energy of a J bond. The argument leads to the phase separation in many hole systems. 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. Thus if J' is sufficiently large ($\sim J/2$), a many-hole cluster should prefer a line shape to the ordinary phase separation. Therefore, the 2nd-neighbor exchange J' can lead to the charge stripe. However, the neutron scattering measurement suggested the four-spin exchange J_4 is more important than J'. In fact the perturbation expansion of the Hubbard Hamiltonian [5] from the large-U limit gave the parameters of the extended t–J model (1) as follows: $J' = J'' = J_4/20 = 4t^4/U^3$. It was also justified by the neutron scattering experiment. Thus we consider the effect of J_4 on the short-range antiferromagnetic order. The realistic positive J_4 stabilizes the triplet state at each four-spin plaquette. It leads to a kind of frustration with the short-range antiferromagnetic order. Thus the stripe formation is more preferable than the phase separation for sufficiently large J_4, because the number of plaquettes where J_4 does not work due to holes is larger for the stripe. Therefore, the four-spin exchange can also be an origin of the charge stripe.

In order to confirm the above mechanism of the stripe, we performed the numerical diagonalization study with the Lanczos algorithm on the extended t–J model (1) on the 4×4 cluster with 4 holes under the periodic boundary condition. In the same study on the t–J–J' model in the previous work, a critical point J'_c was detected as a level cross in the ground state for some realistic values of J/t. The two phases separated by J'_c were characterized by the four-hole correlation functions:

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

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

which are the correlations at four successive sites on a line and at four sites surrounding a plaquette. The numerical calculation indicated $C_{\rm St}^{(4)} < C_{\rm PS}^{(4)}$ for $J' < J'_c$ while $C_{\rm St}^{(4)} > C_{\rm PS}^{(4)}$ for $J' > J'_c$. Thus we concluded that the system exhibits the phase separation for $J' < J'_c$ while the stripe order for $J' > J'_c$.

The present numerical study on the extended t–J model (1) indicated that the same phase transition occurs at some critical value of J_4 even for $J' = J'' = 0$ as the t–J–J' model. It suggests that the four-spin exchange can also lead to the charge stripe. It is expected that for more realistic parameter

$J' = J'' = J_4/20$ the stripe is more stable, because the antiferromagnetic J'' should stabilize the line-shaped hole cluster, based on the same argument as J'. The phase boundaries obtained by the numerical diagonalization study on the 4×4 cluster in the two cases $J' = J'' = J_4/20$ and $J' = J'' = 0$ are shown in Fig. 2. The stripe phase is larger for $J' = J'' = J_4/20$, as expected. The preliminary phase diagram in Fig. 2 suggests that the charge stripe possibly occurs for the realistic parameters $J/t \sim 0.4$ and $J_4 \sim 0.3J(\sim 0.1t)$, which are obtained by the neutron scattering experiment on La_2CuO_4.

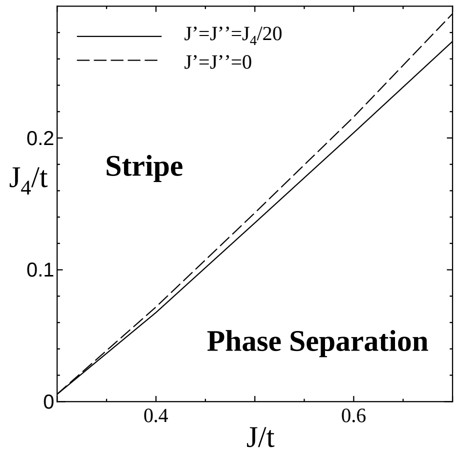

Fig. 2. Ground-state phase diagram.

In summary, the present numerical study on the extended t–J model indicated that the four-spin exchange interaction is possibly one of the origins of the charge stripe in the high-T_c cuprates.

This research was supported by a Grant-in-Aid for Scientific Research from Ministry of Education, Culture, Sports, Science and Technology of Japan.

REFERENCES

[1] M. Tranquada *et al.*, *Nature* **375**, 561 (1995).
[2] S. White, D.J. Scalapino, *Phys. Rev. Lett.*, **80**, 1272 (1998).
[3] T. Sakai, *Phys. Rev.*, **B63**, 140509(R) (2001).
[4] R. Coldea *et al.*, *Phys. Rev. Lett.*, **86**, 5377 (2001).
[5] M. Takahash, *J. Phys.*, **C10**, 1289 (1977).