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

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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 $t' > 0$.

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The charge stripe order \cite{14} 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$_x$Sr$_2$CuO$_4$ \cite{3}, the mechanism of the stripe formation has been studied in many works. The numerical study \cite{4} based on the density matrix renormalization group suggested that such a stripe phase can appear in the two-dimensional $t$-$J$ model. On the other hand, the numerical diagonalization of the $4 \times 4$ $t$-$J$ cluster with two holes \cite{4} 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 $J/t$. \cite{4} The high temperature expansion suggested such a state is realized for $J/t \geq 1$. \cite{8} Some small cluster calculations have shown that a larger cluster of the holes is stable rather than a pair even in more realistic parameter region ($J/t \geq 0.5$). \cite{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$_2$CuO$_2$Cl$_2$ ($t' < 0.3t$) \cite{4}, $J'$ is also expected to be finite in some real cuprates. Thus we consider the square-lattice $t$-$t'$-$J$-$J'$ model to discuss on the mechanism of the stripe.

We also calculate the three- and four-hole correlation functions of the $4 \times 4$ 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

\[
H = -\sum_{i<j,\sigma}^n (\hat{c}_i^\dagger \sigma c_{j,\sigma} + \text{h.c.}) - t' \sum_{i<j,\sigma}^n (\hat{c}_i^\dagger \sigma c_{j,\sigma} + \text{h.c.}) + J \sum_{i<j}^n (\hat{S}_i \cdot \hat{S}_j - \frac{1}{2} n_i n_j) + J' \sum_{i,j,\sigma} (\hat{S}_i \cdot \hat{S}_j - \frac{1}{2} n_i n_j)
\]

where $\sum_{i,j}$ and $\sum_{i,j'}$ 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$_2$CuO$_4$ by the theoretical study based on the \textit{ab initio} calculation. \cite{4} The antiferromagnetic $J'$ term can also be derived from the strong correlation expansion of the Hubbard Hamiltonian up to the order of $t'/U^3$. \cite{4} Since $t'$ plays no essential roles in the following argument, we set $t' = 0$ at 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 $7J$ bonds, while the latter $8$ $J$ 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 (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 than (b). Thus the three hole cluster should prefer the line shape like (a) to the corner shape like (b).

Next we consider the four-hole cluster with the two shapes, shown in Figs.1(c) and (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 the shape (c) than (d). Although 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, the line shape (c) is more preferable than (d) under the condition $J' \geq J/2$. 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 give a possible mechanism of the charge stripe order.

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

3-hole correlation functions

(a) \hspace{1cm} (b)

4-hole correlation functions

(c) \hspace{1cm} (d)

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

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

\[
C_{St}^{(3)} = \langle \sum_i n_i^h n_{i+\hat{x}} n_{i+2\hat{x}} \rangle \quad (2)
\]

\[
C_{PS}^{(3)} = \langle \sum_i n_i^h n_{i+\hat{x}} n_{i+\hat{y}} \rangle \quad (3)
\]

\[
C_{St}^{(4)} = \langle \sum_i n_i^h n_{i+\hat{x}} n_{i+2\hat{x}} n_{i+3\hat{x}} \rangle \quad (4)
\]

\[
C_{PS}^{(4)} = \langle \sum_i n_i^h n_{i+\hat{x}} n_{i+\hat{y}} n_{i+\hat{x}+\hat{y}} \rangle \quad (5)
\]

in the ground state of the finite cluster $t$-$t'$-$J$-$J'$ model ($t' = 0$). $C_{St}^{(3)}$ and $C_{St}^{(4)}$ are supposed to represent a relative strength of the stripe order, while $C_{PS}^{(3)}$ and $C_{PS}^{(4)}$ measure a tendency towards the ordinary phase separation. They are calculated for the $4 \times 4$ cluster with four holes, for which the ground state has the $d$-wave like rotational symmetry for $J \geq 0.3$. \[\] (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 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 $J' \geq J'_c$, while it is reversed for $J' \leq J'_c$ in both Figs. 3 and 4. 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 $t' = 0$ (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 \[\], is stabilized by the next-nearest-neighbor exchange interaction in the upper phase in Fig. 5.

FIG. 3. Three-hole correlation functions versus $J'$ with fixed $J (=0.6$ and $0.8)$.
The phase diagram for $t' = 0$ in Fig. 5 indicates an interesting point that the stripe order is possibly realized even if $J'$ is much smaller than $J/2$ in small-$J$ region around $J \sim 0.4$, which is realistic for the high-$T_c$ cuprates. Some recent theoretical analyses \cite{2,4} 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 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 prese phase boundary is still controversial. Note that the present analysis does not distinguish the static stripe order and the dynamical one like the charge strings, which was predicted by the phonon-induced polaron mechanism. \cite{12,14,15} It would be an interesting future work to study on such a dynamical stripe, which may give some hints to explain the coexistence of

\begin{center}
\begin{figure}[h!]
\centering
\includegraphics[width=0.8\textwidth]{fig4.png}
\caption{Four-hole correlation functions versus $J'$ with fixed $J(=0.6$ and 0.8).}
\end{figure}
\end{center}

\begin{center}
\begin{figure}[h!]
\centering
\includegraphics[width=0.8\textwidth]{fig5.png}
\caption{Phase diagrams in $J'$-$J$ plane for $t'=0$, -0.1 and 0.1.}
\end{figure}
\end{center}

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 \cite{16,17} at least for small $t'$, although they didn’t consider $J'$. It 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 more realistic hole density, close to 1/8, if possible. (For example, the 32-site cluster with 4holes is desirable, but it is difficult for the present computer systems.)

The recent high-resolution inelastic neutron scattering experiment \cite{11} indicated that the ring (four-spin) exchange interaction is more important to explain the observed spin-wave dispersion of La$_2$CuO$_4$, rather than the next-nearest-neighbor exchange interaction. Thus we should also take the ring exchange interaction into account for 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 $4 \times 4$ 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 $t' > 0$.

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