# Stripe States with Spatially Oscillating $d$-Wave Superconductivity in the Two-Dimensional $t$-$t'$-$J$ Model

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We study the interplay between stripes and $d$-wave superconductivity in the two-dimensional $t$-$t'$-$J$ model using a variational Monte Carlo method. The next-nearest-neighbor hopping $t' < 0$ stabilizes the stripe states around $1/8$ hole doping rate. We find that stripes and spatially oscillating superconductivity coexist depending on parameters. The superconducting orders are enhanced at the hole stripe regions. Although the energy differences are relatively small, the stripe state in which the phases between adjacent superconducting stripes are the opposite (antiphase) is also stabilized. We consider the possibility that the antiphase coexistence may explain the weakness of the $c$-axis Josephson couplings in the $La_{1.6-x}Nd_{0.4}Sr_xCuO_4$.

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Stripe states consisting of one-dimensional (1D) charge modulation and incommensurate antiferromagnetic (AF) order have been confirmed experimentally in some high-$T_c$ cuprates [1]. This new type of inhomogeneous state is considered to play a key role in superconductivity. Recent various experiments, such as neutron scattering experiments, muon spin relaxations, and nuclear quadrupole resonances, have revealed that the superconductivity coexists with the static stripe states in $La_{1.6-x}Nd_{0.4}Sr_xCuO_4$ [1–5]. In addition, it is observed by the measurement of optical conductivity [6,7] that the superconductivity in the presence of the static stripe exhibits peculiar properties compared with other cuprates. For example, the penetration depth is 4 times longer than that of the $La_{2-x}Sr_xCuO_4$, and the $c$-axis Josephson plasma edge disappears. To understand these features, it is quite important to elucidate the mechanisms of the stripe formation and the interplay between the stripe states and superconductivity.

Theoretically, there are several issues pertaining to the stripe states. (i) There has been some controversy whether the stripes with periodicity consistent with experiments are realized in microscopic theories such as the Hubbard or $t$-$J$ model [8–13]. Originally the stripe states were found in the mean-field approximation of the Hubbard model [8]. However, the obtained periodicity was twice as long as that observed experimentally. Although this discrepancy can be remedied by introducing the next-nearest-neighbor hopping ($t'$) [9], it is not conclusive since the mean-field theories generally overestimate the AF order. Numerical studies such as the density matrix renormalization group method [11], the exact diagonalization study [12], and the variational Monte Carlo (VMC) method [13] have been applied to the stripe problem in the $t$-$J$ model, but they contradict each other, probably due to the small system size and the boundary effects. (ii) It has often been argued that the stripe state originates from the tendency of the phase separation between the AF state and a hole-rich state [14]. However, the possibility of the phase separation in the small doping region of the two-dimensional (2D) $t$-$J$ model is still controversial [15,16]. (iii) The above studies have taken account of only the 1D charge modulation and the AF order: superconducting (SC) order has not been considered. Although the coexistence of superconductivity and stripes has been discussed phenomenologically in terms of the one dimensionality of stripes [17] and in SO(5) symmetric theory [18], it is a more fundamental issue to study the interplay between the stripes and superconductivity in microscopic models.

In this paper we perform a VMC simulation to investigate competition in energies of various stripe states including states with spatially oscillating $d$-wave SC order parameters. We use the 2D $t$-$t'$-$J$ model, which is considered a realistic model of a $CuO_2$ plane of high-$T_c$ cuprates. In the VMC method, we can study the above issues using fairly large system sizes and treating the exclusion of double occupancies rigorously. We clarify that (i) the stripe state, consistent with experiments, is stabilized when the next-nearest-neighbor hopping term $t'$ is introduced, whose sign ($t' < 0$) reproduces the actual Fermi surface of cuprates, and that (ii) the tendency to phase separation does not stabilize the stripe state. (iii) We also consider the possibility of stripe states with superconductivity. We find that the stripe state with spatially oscillating SC order parameters is stabilized depending on parameters, although the variational energy is close to that of the stripe state without SC order.

The obtained superconductivity in the stripe state can have a peculiar character: there is a $\pi$ phase shift between the adjacent hole stripes. This will explain the suppression of the $c$-axis Josephson coupling. We also discuss the possible origin of this $\pi$ phase shift from the viewpoint of Josephson couplings between SC stripes.

  

We use the 2D $t$-$t'$-$J$ model on a square lattice,

$$H = -t \sum_{\langle ij \rangle \sigma} P_{\mathrm{G}}(c_{i\sigma}^{\dagger} c_{j\sigma} + \mathrm{H.c.}) P_{\mathrm{G}} - t' \sum_{\langle\langle ij \rangle\rangle \sigma} P_{\mathrm{G}}(c_{i\sigma}^{\dagger} c_{j\sigma} + \mathrm{H.c.}) P_{\mathrm{G}} + J \sum_{\langle ij \rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_j , \tag{1}$$

where $\langle ij \rangle$ and $\langle\langle ij \rangle\rangle$ represent the sums over the nearest-neighbor and next-nearest-neighbor sites, respectively. $c_{i\sigma}^{\dagger}$ ($c_{i\sigma}$) is a creation (annihilation) operator of the spin $\sigma$ ($\uparrow$ or $\downarrow$) electron at site $i$ and $\boldsymbol{S}_i = c_{i\alpha}^{\dagger}(\frac{1}{2}\boldsymbol{\sigma})_{\alpha\beta} c_{i\beta}$. Gutzwiller's projection operator $P_{\mathrm{G}}$ is defined as $P_{\mathrm{G}} = \Pi_i(1 - \hat{n}_{i\uparrow}\hat{n}_{i\downarrow})$, where $\hat{n}_{i\sigma} = c_{i\sigma}^{\dagger} c_{i\sigma}$.

As trial states with stripes, we use Gutzwiller-projected mean-field–type wave functions $P_{N_e} P_{\mathrm{G}} |\phi_0\rangle$ with fixing the number of electrons $N_e$ through $P_{N_e}$. $|\phi_0\rangle$ is constructed as a vacuum of a mean-field Hamiltonian,

$$H_{\mathrm{MF}} = \sum_{ij} (c_{i\uparrow}^{\dagger} c_{i\downarrow}) \begin{pmatrix} H_{ij\uparrow} & F_{ij} \\ F_{ji}^{*} & -H_{ji\downarrow} \end{pmatrix} \begin{pmatrix} c_{j\uparrow} \\ c_{j\downarrow}^{\dagger} \end{pmatrix}, \tag{2}$$

with

$$H_{ij\sigma} = -t \sum_{\delta^{\mathrm{N}}} \delta_{j,i+\delta^{\mathrm{N}}} - t'_v \sum_{\delta^{\mathrm{NN}}} \delta_{j,i+\delta^{\mathrm{NN}}} + [-\mu + \rho_i + \mathrm{sgn}(\sigma)(-1)^{x_i+y_i} m_i] \delta_{ij} , \tag{3}$$

$$F_{ij} = \sum_{\delta^{\mathrm{N}}} \Delta_{ij} \delta_{j,i+\delta^{\mathrm{N}}} . \tag{4}$$

Here $\delta^{\mathrm{N}}$ and $\delta^{\mathrm{NN}}$ are vectors toward the nearest-neighbor and the next-nearest-neighbor sites, respectively, and $\mathrm{sgn}(\sigma) = 1$ or $-1$ according to $\sigma =\uparrow$ or $\downarrow$. In order to introduce stripe configurations, we assume spatially oscillating $\rho_i$ and $m_i$. Their explicit forms are chosen as

$$\rho_i = \rho \cos[2\boldsymbol{q}(\boldsymbol{r}_i - \boldsymbol{r}_0)], \tag{5}$$

$$m_i = m \sin[\boldsymbol{q}(\boldsymbol{r}_i - \boldsymbol{r}_0)], \tag{6}$$

where $\boldsymbol{q} = (0, 2\pi\delta)$ with $\delta$ being the hole doping rate. The amplitudes $\rho$ and $m$ are variational parameters. $\boldsymbol{r}_0 = 0$ corresponds to the site-centered stripe and $\boldsymbol{r}_0 = (0, \frac{1}{2})$ to the bond-centered stripe. For the case $\boldsymbol{r}_0 = 0$, adjacent stripes containing holes are located at $y_i = 0$ and $1/2\delta$ and run along the $x$ direction. Since it is expected that the SC order is enhanced on the hole stripes, we assume the following two types of spatial variations of $\Delta_{ij}$.

(A) antiphase:

$$\begin{aligned} \Delta_{i,i+\hat{x}} &= \Delta_d \cos[\boldsymbol{q}(\boldsymbol{r}_i - \boldsymbol{r}_0)], \\ \Delta_{i,i+\hat{y}} &= -\Delta_d \cos[\boldsymbol{q}(\boldsymbol{r}_i + (0, \tfrac{1}{2}) - \boldsymbol{r}_0)], \end{aligned} \tag{7}$$

(B) in phase:

$$\begin{aligned} \Delta_{i,i+\hat{x}} &= \Delta_d |\cos[\boldsymbol{q}(\boldsymbol{r}_i - \boldsymbol{r}_0)]| , \\ \Delta_{i,i+\hat{y}} &= -\Delta_d |\cos[\boldsymbol{q}(\boldsymbol{r}_i + (0, \tfrac{1}{2}) - \boldsymbol{r}_0)]| . \end{aligned} \tag{8}$$

Here $\Delta_d$ is another variational parameter. Although the in-phase SC order parameter has usually been considered, we will show that the antiphase order parameter is stabilized depending on parameters.

To obtain the ground state $|\phi_0\rangle$, we diagonalize the Hamiltonian in Eq. (2) (the Bogoliubov–de Gennes equation) to obtain $N$ positive eigenvalues $E_\alpha$ ($\alpha = 1 - N$) and $N$ negative eigenvalues $\bar{E}_\alpha$ with corresponding eigenvectors $(u_i^\alpha, v_i^\alpha)$ and $(\bar{u}_i^\alpha, \bar{v}_i^\alpha)$. Using these eigenvectors we have the Bogoliubov transformations

$$\gamma_\alpha = u_i^\alpha c_{i\uparrow} + v_i^\alpha c_{i\downarrow}^{\dagger} \qquad (E_\alpha > 0), \tag{9}$$

$$\bar{\gamma}_\alpha = \bar{u}_i^\alpha c_{i\uparrow} + \bar{v}_i^\alpha c_{i\downarrow}^{\dagger} \qquad (\bar{E}_\alpha < 0), \tag{10}$$

and then $|\phi_0\rangle$ can be constructed by creating all negative energy states and annihilating all positive energy states on a vacuum of electrons $|0\rangle$, i.e., $|\phi_0\rangle = \prod_\alpha \gamma_\alpha \bar{\gamma}_\alpha^{\dagger} |0\rangle$.

Using the above wave function we calculate expectation values of various physical quantities by means of the VMC method. An expectation value of an operator $\hat{O}$ is

$$\langle \hat{O} \rangle \equiv \frac{\langle \phi_0 | P_{\mathrm{G}} \hat{O} P_{\mathrm{G}} | \phi_0 \rangle}{\langle \phi_0 | P_{\mathrm{G}} P_{\mathrm{G}} | \phi_0 \rangle} . \tag{11}$$

We calculate the variational energy $E_{\mathrm{var}} = \langle H \rangle$ of the Hamiltonian (1) to obtain the optimized state. We perform this calculation on the $N_x \times N_y$ square lattice with 100–288 sites. Here $N_x$ and $N_y$ are the number of sites in the $x$ and $y$ direction, respectively. It is found that the energy of the inhomogeneous state is sensitive to the choice of boundary conditions, i.e., periodic or antiperiodic with respect to the hopping terms. To reduce the boundary condition dependences, we average the energies over the four different sets of boundary conditions with periodic or antiperiodic ones in each direction. This kind of procedure is known to be effective in numerical studies, such as small-cluster exact diagonalization [19,20]. In the 1D $t$-$J$ model, this method gives a quite good result for the ground state energy [20].

Figure 1 shows the $t'$ dependences of the optimized variational energies at $J/t = 0.3$ for various system sizes. The hole doping rates $\delta$ are $1/8$ [see Fig. 1(a)] and $1/10$ [see Fig. 1(b)]. The solid symbols in Fig. 1(a) show the system size dependence of the variational energy for the stripe states without SC order. As we increase the number of sites, the size dependence becomes weak and we clearly see that the stripe state has a lower variational energy than the homogeneous $d$-wave SC state (expressed by $\times$ symbols) when $t'/t < -0.1$ for $\delta = 1/8$. The same result is obtained for $\delta = 1/10$ when $t'/t < -0.2$ [Fig. 1(b)].

Here we discuss the effect of the $t'$ term on the stripe formation. Without $t'$ term, any stripe states give higher energy than the homogeneous $d$ wave state. This means that the negative $t'$ is necessary for stabilizing the stripe states. We consider several reasons: (i) It is known that holes can be doped in the AF region when $t' > 0$. However, holes are repelled out from the AF region when $t' < 0$, which leads to the stripe formation. (ii) The nesting property of the Fermi surface, discussed in the Hubbard model [9], also helps the stabilization of the stripe states with the present incommensurability. In our calculation, it is apparent that

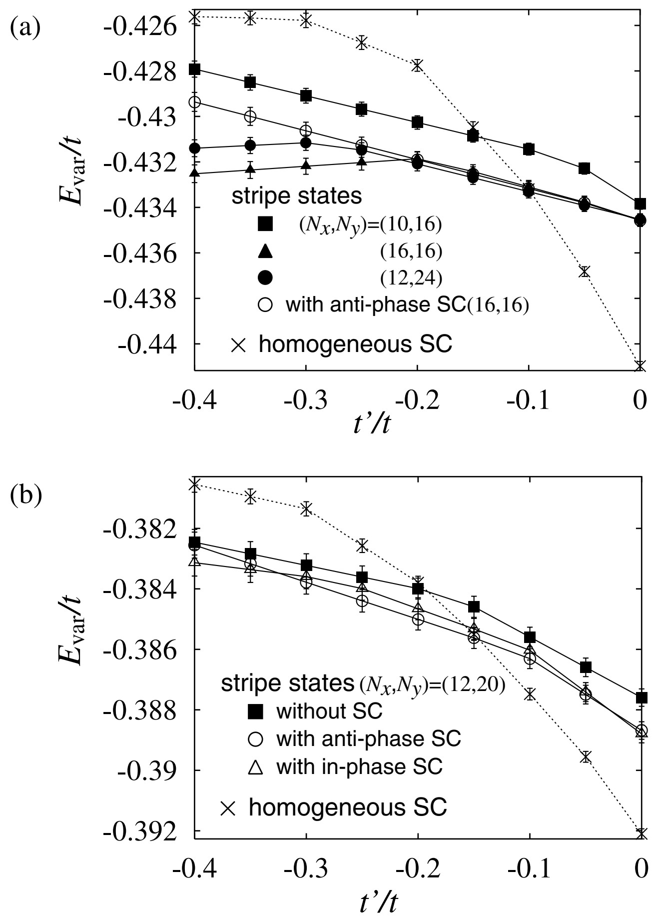


FIG. 1. Variational energies of the stripe states for $J/t = 0.3$: (a) 1/8 doping and (b) 1/10 doping as a function of $t'/t$. The data have been optimized with respect to the parameters $\rho$, $m$, $t'_v$, $\mu$, and $\Delta_d$. The filled symbols represent the energies of the stripe states without SC order. The open symbols indicate those of the stripe states with antiphase (open circles) and in-phase (open triangles) SC order. Energies of the homogeneous $d$-wave superconducting states are shown by the × symbols.

the stripe stability is sensitive to $t'/t$ which determines the geometry of the Fermi surface.

Let us discuss the relation to the phase separation. It has been shown [21] that the negative $t'$ term suppresses the tendency toward the phase separation. We have confirmed this in our VMC calculations. Considering these effects of the negative $t'$ term, we conclude that the tendency to phase separation does not favor the stripe formation. Our results are also consistent with Han *et al.* [22] who showed that the suppression of the phase separation with a Coulomb repulsion stabilized the stripe states. In order to check this further, we carried out VMC calculations at larger values of $J/t$ ($J/t = 0.5$), where the tendency of the phase separation is stronger. In this large $J/t$ region, the stripe states are not stabilized for $\delta = 1/8$ and $1/10$.

Next we study the interplay between the stripe states and superconductivity. In Fig. 1, we also show the variational energies of the stripe states *with* SC order parameters (open symbols). For $\delta = 1/8$ [Fig. 1(a)], the variational energy of the stripe state with SC order is slightly higher than that without SC order, while it is the lowest variational energy for $\delta = 1/10$ and $t'/t < -0.15$ [Fig. 1(b)]. Although both coexistent states with in-phase and antiphase SC have similar energies in Fig. 1(b), the state with antiphase SC order is slightly stabilized.

These calculations show that the coexistent states of stripes and SC order are stable in certain parameters. However, the energy gains $\sim 0.001t$ are small in the parameter region appropriate for high-$T_c$ cuprates (probably $t'/t = -0.1 \sim -0.3$). Considering the size and boundary condition dependences, we speculate that, in the $t$-$t'$-$J$ model, there are various low-energy states including stripe states with and without SC order parameters. This type of quasi-degeneracy occurs specifically for $t'/t = -0.1 \sim -0.3$ and the doping rate $\delta = 1/8$ and $1/10$. This is the reason why the previous numerical studies have been controversial [11,12]. In the actual high-$T_c$ materials, we expect that the state is sensitive to small perturbations, such as low temperature tetragonal lattice distortions in La-based cuprates. Our finding will also explain the variety of $T_c$ near $\delta = 1/8$ in LSCO [23].

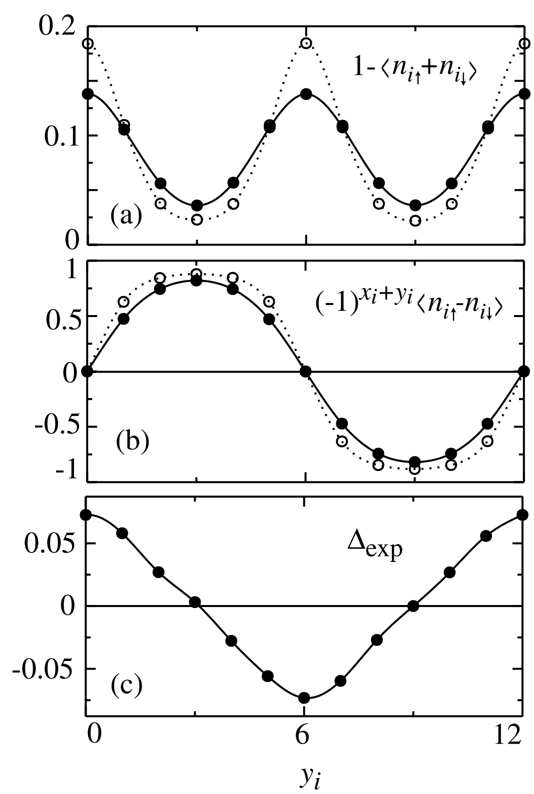


FIG. 2. Profiles of the expectation values of (a) hole density $1 - \langle n_{i\uparrow} + n_{i\downarrow}\rangle$, (b) staggered magnetization $(-1)^{x_i+y_i}\langle n_{i\uparrow} - n_{i\downarrow}\rangle$, and (c) the $d$-wave SC order parameters are plotted (solid circles) in the optimized variational state in the $t$-$t'$-$J$ model with $J/t = 0.3, t'/t = -0.15$. The hole density is chosen as $\delta = 1/12$, but similar profiles are also obtained for $\delta = 1/8$, where the distance of the adjacent hole stripes is four lattice constants consistent with experiments. For comparison, profiles in the optimized stripe state without $d$-wave SC order ($\Delta_d = 0$) are also shown by the open circles.

The stripe state with the antiphase SC order parameter found here is a new exotic state. In Fig. 2, we show the spatial variation of the expectation values in this state for $\delta = 1/12$, $t'/t = -0.15$, and $J/t = 0.3$ (solid circles). For comparison, those in the stripe states without SC order are shown as open circles. Stripes are located along the $x$ direction, where the hole density is large, and the neighboring stripes are separated by the regions with the enhanced staggered magnetization. It is noted that the hole density in the stripe is about 0.14 which is much smaller than 0.5 in the schematic picture originally proposed [1]. This is due to the apparent quantum fluctuation of the stripes. In comparison to the stripes without $d$-wave SC order (open circles), the AF domain wall and hole stripes are not as sharp. Also the maximum of the staggered magnetization is slightly suppressed due to the presence of $d$-wave SC orders. In Fig. 2(c), we show the spatial variation of the SC order parameter $\Delta_{\exp}$ obtained from the calculations of the correlation functions,

$$D_x(\boldsymbol{i}, \boldsymbol{i} + \boldsymbol{l}) = \sum_{\sigma} \langle c_{i\sigma}^{\dagger} c_{i+\hat{x},-\sigma}^{\dagger} c_{i+l+\hat{x},-\sigma} c_{i+l,\sigma} \rangle . \quad (12)$$

It is shown that the $d$-wave SC order is enhanced along the hole-rich region. The maximum value of $\Delta_{\exp}$ on the stripes is close to the value in the homogeneous $d$-wave SC state which has $\Delta_{\exp} = 0.058$.

Now we discuss why the antiphase SC order is stabilized. It is known that indirect tunneling through an Anderson magnetic impurity produces the negative Josephson coupling [24]. It is explained as follows: Because of the prohibition of the double occupancy, a Cooper pair tunneling though the impurity must accompany an exchange of one electron of the pair with the impurity electron. This process gives an extra sign $(-1)$ for the Josephson coupling due to the anticommutation relation of fermions. In our case, we speculate that an indirect tunneling process across the magnetic AF domain without double occupancy stabilizes the $\pi$ phase shift between neighboring SC stripes through the negative Josephson coupling. Further work would, however, be needed to study carefully the difference between the AF domain and single magnetic impurity.

We find that the qualitative differences between stripe states with in-phase SC order and with antiphase SC order do not appear in the spatial profile and the momentum distribution function. However, the difference will appear if we perform phase sensitive experiments such as the Josephson plasma resonance. In fact, it is reported that the $c$-axis Josephson plasma edge disappears in $La_{1.6-x}Nd_{0.4}$-$Sr_xCuO_4$ [6]. We believe this disappearance could be explained by the stripe states with the antiphase SC order. Because the direction of the stripes are rotated by 90° in the neighboring $CuO_2$ planes, the Josephson coupling is drastically weakened compared with the in-phase SC states due to the phase alternations.

In the actual experimental situations at finite temperatures and with disorders, we expect that the phases between adjacent hole stripes can be in-phase or antiphase at random because the energy difference is small. This also weakens the superconductivity in stripe states.

In summary, we investigate the stability of the stripe states for $t'/t < 0$ and the coexistence with the $d$-wave SC order in the 2D $t$-$t'$-$J$ model. We found that the stripe state is stabilized near 1/8 doping if we introduce the negative $t'$ term, while this term does not favor the phase separation. It is found that the stripe states with antiphase SC, which have not been considered before, are slightly stabilized compared with the stripes with in-phase SC. We consider that such an antiphase SC order explains the weakness of the $c$-axis Josephson coupling.


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