Interplay between staggered flux and $d$-wave superconducting orders in $t$-$t'$-$J$ model

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Abstract. With cuprate superconductors in mind, we check whether the $d$-wave superconducting ($d$SC) state coexists with or excludes the staggered flux (SF) state, which was revealed to be a strong candidate for the pseudogap state. To this end, we use a variational Monte Carlo method for the square-lattice $t$-$J$ model with diagonal transfer $t'$. We construct a trial wave function which can simultaneously represent $d$SC and SF orders for a continuous description of their interplay. Furthermore, a band renormalization effect is introduced into both orders independently. It is found that the SF state does not coexist with $d$SC and is unstable for a wide area in the parameter space. However, a strange state having both SF and antiferromagnetic orders is found to be stable for very low doping rate.

1. Introduction

In research for understanding superconductivity (SC) in high-$T_c$ cuprates, what is the origin of pseudogap phenomena, which behave like a shadow of SC, has been a long-standing problem [1, 2]. A staggered flux (SF) state is one of the likely candidates for the pseudogap state proposed so far: Using a variational Monte Carlo (VMC) method, it was revealed that the SF state has properties consistent with the behavior of the pseudogap phase in cuprates and is moderately stable for the $t$-$J$ model [3], and for the Hubbard model with diagonal transfer $t'$ [4]. In the latter, it is shown that the SF state becomes more stable than the normal state (projected Fermi sea) for a strongly correlated and underdoped area, although the $d_{x^2-y^2}$-wave SC ($d$SC) state always has lower energy. Especially, for $t'/t \sim -0.3$, the area where the SF state is more stable than the normal state expands in a wide doping range, and the energy of SF state approaches that of $d$SC. Meanwhile, coexistence or exclusivity of the $d$SC gap and the pseudogap has been debated, and some recent experiments reported coexistence of the two gaps [5].

Thus, it is important to check whether the SF and $d$SC orders coexist or are mutually exclusive. In the preceding study [6], we directly checked this problem using a mixed state of the SF and $d$SC orders, by applying a VMC method to the Hubbard ($t$-$t'$-$U$) model. It revealed that the SF order competes with the $d$SC order and is not stabilized. In Ref. [6], however, band renormalization effect (BRE) is introduced only into the SC order. If BRE is introduced into SC and SF orders independently, the result will possibly change. Another problem is that the Hubbard model is possibly lacking in some important elements for describing cuprates because the antiferromagnetic (AF) state (or phase separation) becomes stable against $d$SC for a wide
area in the model-parameter space [7]. In this context, it is significant to check whether or not the t-J model exhibits essentially similar behavior as an effective model in a large-\(U/t\) regime.

In this work, we will check these points by applying a VMC method with a mixed state of SF and dSC orders, which includes individual BRE for both orders, to a \(t-t' - J\) model with three-site hopping \(J^{(3)}\). On the basis of the data of the optimized states, we found that the SF and dSC orders are mutually exclusive in a wide area of the parameter space, and the SF order does not appear in the ground state. As an exception, for \(J^{(3)}/J = -1\) near half-filling, a coexisting state of SF and AF becomes stable and dSC order vanishes. This extraordiary state has properties relevant to the present topics.

2. Method

We consider a \(t-J\) model on the square lattice with the diagonal transfer (\(t'\)) and the three-site \((J^{(3)})\) terms:

\[
H_{\text{tot}} = H_t + H_{t'} + H_J + H_{J^{(3)}}
\]

\[
= -t \sum_{\langle rr' \rangle, \sigma} \left( \hat{c}_{r,\sigma}^\dagger \hat{c}_{r',\sigma} + \text{h.c.} \right) - t' \sum_{\langle rr' \rangle, \sigma} \left( \hat{c}_{r,\sigma}^\dagger \hat{c}_{r',\sigma} + \text{h.c.} \right) + J \sum_{\langle rr' \rangle} \left( \mathbf{S}_r \cdot \mathbf{S}_{r'} - \frac{1}{4} n_r n_{r'} \right)
\]

\[
- \frac{J^{(3)}}{4} \sum_{\tau, \tau' \neq \tau} \left( \hat{c}_{\tau,\sigma}^\dagger \hat{c}_{\tau'-\tau,\sigma} \hat{c}_{\tau+\tau',\sigma} + \hat{c}_{\tau+\tau',-\sigma} \hat{c}_{\tau'-\tau,\sigma} \hat{c}_{\tau,\sigma}^\dagger \hat{c}_{\tau+\tau',\sigma} \right),
\]

where \(\hat{c}_{r,\sigma}^\dagger = c_{r,\sigma}^\dagger(1 - n_{r,\sigma})\), \(\hat{c}_{r,\sigma}\) creates an electron of spin \(\sigma\) at site \(r\), \(n_r = \sum_\sigma n_{r,\sigma} = \sum_\sigma c_{r,\sigma}^\dagger c_{r,\sigma}\), and \(\mathbf{S}_r = \frac{1}{2} \sum_\sigma \sum_{\sigma'} c_{r,\sigma}^\dagger c_{r,\sigma'} \sigma_\sigma'^{(\text{Pauli})}\) with \(\sigma = (\sigma_x, \sigma_y, \sigma_z)\) being the vector of Pauli matrices. \((\mathbf{r}, \mathbf{r}')\) and \((\mathbf{r}'', \mathbf{r}''')\) denote indices of nearest-neighbor and diagonal-neighbor pairs, respectively. Note that \(H_{\text{tot}}\) works in the space with no double occupancy. The three-site term \(H_{J^{(3)}}\), in which \(\tau, \tau' = (\pm 1, 0), (0, \pm 1)\) with the unit of length being the lattice constant, is often disregarded but may be significant in comparing with the Hubbard model; \(H_{J^{(3)}}\) is the same order as \(H_J\) in the \(t/U\) expansion with \(J = 4t^2/U\) and \(J^{(3)} = J\), corresponding to electron-doped cases [8]. On the other hand, it was argued that \(J^{(3)}/J\) could be negative for hole-doped cases [9, 10]. Therefore, in this work, we treat \(J^{(3)}\) as a model parameter independent of \(J\).

To this model, we apply a VMC method using the correlated measurement for efficient optimization [11]. We use a Jastrow-type trial wave function, \(\Psi = \mathcal{P}^C \mathcal{P}^S \Phi\), where \(\mathcal{P}^C\) and \(\mathcal{P}^S\) are intersite correlation factors of Jastrow-type for charge and spin, respectively:

\[
\mathcal{P}^C = \prod_{rr', \sigma, \sigma'} \left[ 1 - \{ 1 - \eta^C (|r - r'|) \} n_{r,\sigma} n_{r',\sigma'} \right],
\]

and

\[
\mathcal{P}^S = \prod_{rr'} \left[ 1 - \{ 1 - \eta^S (|r - r'|) \} S^z_r S^z_{r'} \right],
\]

with \(S^z_r = \frac{1}{2} (n_{r,\uparrow} - n_{r,\downarrow})\). To exclude double occupancy, we impose the condition \(\eta^C(0) = 0\).

For a short-range part of charge correlations, we consider up to the fourth-neighbour sites as illustrated in Fig. 1(b): \(\eta^C = \eta^C (|r - r'|)\) for \(1 \leq \ell \leq 4\) is an independent variational parameter. For long-range correlations, we assume a Tomonaga-Luttinger-liquid form [8, 12],

\[
\eta^C (|r - r'|) = \left[ \frac{L}{\pi} \sin^2 \left( \frac{\pi x}{L} \right) + \sin^2 \left( \frac{\pi y}{L} \right) \right]^\nu \quad \text{for} \quad \sqrt{5} < |r - r'|,
\]

where \(r - r' = (x, y)\) and \(L\) is a linear dimension of the square lattice composed of \(L \times L\) (\(= N_s\)) sites. A variational parameter \(\nu\) in Eq. (4) works as repulsive (attractive) correlation for \(\nu > 0\)
For spin part $P^S$, correlations up to the tenth-neighbor sites are taken into account: 

$$
\eta^S_\ell = \eta^S_\ell (|r - r'|) \text{ for } 1 \leq \ell \leq 10 \text{ is an independent variational parameter, and spin correlations for } 11 \leq \ell \text{ are disregarded.}
$$

For the one-body part $\Phi$, we adopt a mixed state of SF and $d$SC for a continuous description of their interplay. For $N_e$ electrons, $\Phi$ with a nearest-neighbor-pairing gap $\Delta_d$ is written as [13],

$$
\Phi = \left( \sum_k \sum_{\lambda = \pm} \varphi_k \alpha^\dagger_{\lambda, k, \uparrow} \alpha^\dagger_{\lambda, -k, \downarrow} \right) \frac{N_e}{2} |0\rangle ,
$$

where

$$
\varphi_k = \frac{\Delta(k)}{\epsilon^{SC}(k) - \zeta + \sqrt{(\epsilon^{SC}(k) - \zeta)^2 + |\Delta(k)|^2}} ,
$$

with $\Delta(k) = \Delta_d (\cos k_x - \cos k_y)$.

$\alpha^\dagger_{\lambda, k, \sigma}$ in Eq. (5) is a creation operator of a quasi-particle in SF state that is constructed by diagonalizing a SF Hamiltonian $H^{SF}$ as follows. The noninteracting SF Hamiltonian with transfers up to the fifth-neighbor sites in the sublattice (A, B) representation, shown in Fig. 1, is written as [4],

$$
H^{SF}(\theta) = \sum_{k, \sigma} \left( \alpha^\dagger_{k, \sigma} b_{k, \sigma} \right) \begin{pmatrix}
\varepsilon^{SF}_2(k) + \varepsilon^{SF}_3(k) & \frac{u(k, \theta)}{\varepsilon^{SF}_2(k) + \varepsilon^{SF}_3(k)} \\
\frac{\varepsilon^{SF}_2(k) + \varepsilon^{SF}_3(k)}{u^*(k, \theta)} & \varepsilon^{SF}_2(k) + \varepsilon^{SF}_3(k)
\end{pmatrix} \begin{pmatrix}
\alpha_{k, \sigma} \\
\beta_{k, \sigma}
\end{pmatrix} ,
$$

where $\theta$ is the phase of local circular current in SF state, $a_{k, \sigma} (b_{k, \sigma})$ is a Fourier transformation of an annihilation operator on a sublattice A (B),

$$
u(k, \theta) = -2 t_{1x}^{SF} e^{i\theta} \cos k_x - 2 t_{1y}^{SF} e^{-i\theta} \cos k_y + \varepsilon^{SF}_4(k) + \varepsilon^{SF}_5(k) ,
$$

Figure 1. (a) Schematic figure of the staggered flux state. Arrows denote the local circular current, which flows in alternate directions in each plaquette. (b) Definition of variational parameters, which are classified by intersite distance: Band parameters $t^X_\ell$ for optimizing $\varepsilon^X(k)$ with $X = SF$ or SC, and intersite correlation parameters $\eta^Y_\ell$ in $P^Y$ with $Y = C$ or S.
tight-binding band composed of transfers up to fifth-neighbor sites as shown in Fig. 1(b), "different from the SF one. To this end, we assume that to be optimized together with the other parameters.

\[ \varepsilon_X^X(k) = -4t_X^X \cos k_x \cos k_y, \]
\[ \varepsilon_X^Y(k) = -2t_X^Y \cos(2k_x) + \cos(2k_y), \]
\[ \varepsilon_X^Z(k) = -4t_X^Z \cos(2k_x) \cos(k_y) + \cos(k_x) \cos(2k_y), \]
\[ \varepsilon_X^5(k) = -2t_X^5 \cos(3k_x) + \cos(3k_y). \]  
(9)

with \( X = SF \). Note that the phase \( \theta \) is accompanied by only the nearest-neighbor transfer \( t_{1x}^{SF} \) but not by \( t_{1x}^{SF} - t_{1y}^{SF} \), and asymmetry in \( t_{1x}^{SF} \) is also introduced between \( x \) and \( y \) directions (\( t_{1x}^{SF} \) and \( t_{1y}^{SF} \)) to deal with the Pomeranchuk instability [14].

By applying a Bogoliubov transformation,
\[ a_{k,\sigma} = \frac{\Gamma(k, \theta)}{\sqrt{2}} (-\alpha_{-k,\sigma} + \alpha_{+k,\sigma}), \quad b_{k,\sigma} = \frac{1}{\sqrt{2}} (\alpha_{-k,\sigma} + \alpha_{+k,\sigma}), \]  
(10)

with
\[ \Gamma(k, \theta) = \frac{u(k, \theta)}{S(k, \theta)}, \quad S(k, \theta) = \sqrt{u(k, \theta) u^*(k, \theta)}, \]  
(11)

\[ u(k, \theta) u^*(k, \theta) = 4 \left( \left( t_{1x}^{SF} \cos k_x \right)^2 + \left( t_{1y}^{SF} \cos k_y \right)^2 + 2t_{1x}^{SF} t_{1y}^{SF} \cos(2\theta) \cos k_x \cos k_y \right) - 4 \cos \theta \left( t_{1x}^{SF} \cos k_x + t_{1y}^{SF} \cos k_y \right) \left[ \varepsilon_{4}^{SF}(k) + \varepsilon_{5}^{SF}(k) \right] + \left[ \varepsilon_{4}^{SF}(k) + \varepsilon_{5}^{SF}(k) \right]^2, \]  
(12)

\( \mathcal{H}^{SF}(\theta) \) in Eq. (7) is diagonalized as
\[ \mathcal{H}^{SF}(\theta) = \sum_{k,\sigma} \sum_{\lambda = \pm} \varepsilon_{\lambda}^{SF}(k, \theta) \alpha_{\lambda,k,\sigma} \alpha_{\lambda,k,\sigma}^{\dagger}, \]  
(13)

where the upper and lower band dispersions are given by,
\[ \varepsilon_{\pm}^{SF}(k, \theta) = \pm S(k, \theta) + \varepsilon_{4}^{SF}(k) + \varepsilon_{5}^{SF}(k). \]  
(14)

Corresponding creation operators of the quasi-particle for the upper and lower band, which constitute Cooper pairs in Eq. (5), are obtained by the inverse transformation of Eq. (10) as
\[ \alpha_{\pm,k,\sigma}^{\dagger} = \frac{1}{\sqrt{2}} \left( \pm \Gamma(k, \theta) a_{k,\sigma}^{\dagger} + b_{k,\sigma}^{\dagger} \right), \]  
(15)

where the phase \( \theta \), which is introduced into Eq. (5) through \( \alpha_{\lambda,k,\sigma}^{\dagger} \), is a variational parameter to be optimized together with the other parameters.

In addition, BRE owing to electron correlation is separately introduced into the SC dispersion different from the SF one. To this end, we assume that \( \varepsilon^{SC}(k) \) in Eq. (6) is fitted by another tight-binding band composed of transfers up to fifth-neighbor sites as shown in Fig. 1(b),
\[ \varepsilon^{SC}(k) = -2(t_{1x}^{SC} \cos k_x + t_{1y}^{SC} \cos k_y) + \sum_{i=2}^{5} \varepsilon_{i}^{SC}(k), \]  
(16)

where \( \varepsilon_{i}^{SC}(k) \) is given in Eq. (9) with \( X = SC \), and asymmetry in \( t_{1x}^{SC} \) between \( x \) and \( y \) directions is introduced again for the Pomeranchuk instability.

Hopping parameters in \( \varepsilon^{SC}(k) \) and \( \varepsilon_{\pm}^{SF}(k, \theta) \) are optimized for BRE with some exceptions: \( t_{1x}^{X} \) (\( X = SF \) and \( SC \)) is fixed to \( t \) in Eq. (1) as the unit of energy, and \( t_{1x}^{SF} \) and \( t_{3}^{SF} \) included
in the diagonal elements in Eq. (7) are disregarded because of difficulties in the optimization procedure.

As a result, variational parameters to be optimized in $\Phi$ amount to $\Delta_d, \zeta, \theta, \ell_{1y}^{SC}, \ell_{2}^{SC}, \ell_{5}^{SC}, \ell_{1y}^{SF}, \ell_{4}^{SF}$, and $\ell_{5}^{SF}$. Besides these eleven in $\Phi$, variational parameters in the correlation factors are $\eta_{C}^{\ell}$ for $\ell = 1$-4 and $\nu$ in $P^{C}$, and $\eta_{S}^{\ell}$ for $\ell = 1$-10 in $P^{S}$. According to a standard procedure of VMC, we obtain the optimal set of the 26 parameters by minimizing the energy. Using the optimized wave functions, we calculate various quantities. Among them, we mainly discuss the following order parameters of respective orders. For $d$SC, we use the real-space $d_{x^2-\gamma^2}$-wave SC correlation function for the nearest-neighbor pairing defined by,

$$P_d(r) = \frac{1}{N_{s}} \sum_{\tau, \tau'} \lambda_{xy}(\tau) \lambda_{xy}(\tau') \langle \Delta^{\dagger}(\tau') + \Delta(\tau) \rangle,$$

with

$$\Delta(\tau, \tau') = \frac{1}{\sqrt{2}} \left( c_{\tau\uparrow} c_{\tau\downarrow} - c_{\tau\downarrow} c_{\tau\uparrow} \right),$$

$\lambda_{xy}(\tau) = +1$ for $\tau = (\pm 1, 0)$, and $\lambda_{xy}(\tau) = -1$ for $\tau = (0, \pm 1)$. Actually, we show $P_d(r)$ at the farthermost distance $r = (L/2, L/2)$ as a measure of $d$SC order. For the SF phase, we employ the circular current defined as,

$$J_c/t = \frac{1}{N_{s}} \sum_{r \in A, \sigma} \sum_{\tau} \lambda_{xy}(\tau) \Im \langle c_{\tau+\tau, \sigma}^\dagger c_{\tau, \sigma} - c_{\tau, \sigma}^\dagger c_{\tau+\tau, \sigma} \rangle.$$

(18)

The staggered magnetization,

$$m_s = \frac{1}{N_{s}} \left| \sum_{r} e^{iQ \cdot r} \langle S_{r}^z \rangle \right|,$$

(19)

with $Q = (\pi, \pi)$ is also calculated as the order parameter of AF state.

As pilot calculations, $J/t$ and $t'/t$ are fixed at typical values of hole-doped cuprates, 0.3 and $-0.3$, respectively, and we compare the results of several values of $J^{(3)}/J$ for systems of $L = 10$ and $L = 12$ with periodic-antiperiodic boundary conditions.

3. Results and discussion

Let us begin with the expectation values of energy components (Fig. 2) and order parameters (Fig. 3), estimated by the optimized $\Psi$. In almost the whole range of the present calculations, the circular current $|J_c|/t$ and staggered magnetization $m_s$ vanish, but the pair correlation function $P_d(L/2, L/2)$ has finite values, and monotonically increases as $\delta$ increases within $\delta \leq 0.2$. Thus the pure $d$SC is realized, and robust as compared to the strongly correlated Hubbard model.

The SF order is totally suppressed in a wide range of model parameters. This is explained, by considering $E_{dSC} < E_{SF}$, as follows: The predominant $d$SC state opens a gap in the momentum space except for $k_x = k_y$, whereas the subordinate SF state needs to have a finite pocket Fermi surface (FS) around $k = (\pi/2, \pi/2)$ [4]. Thus, the requirements of the two electronic states do not meet. Including the exceptional case discussed below, the $d$SC order and the SF and AF (type-II in Ref. [7]) orders are mutually exclusive. The overall feature is consistent with that in the Hubbard model of $U/t = 12$ [6].

An exception occurs for $J^{(3)}/J = -1$ and very low doping rate ($\delta \sim 0.03$), where extraordinary behavior appears both in energy components and order parameters, as seen in Figs. 2(c) and 3(c), respectively. A kink appear in each energy component, and $|J_c|/t$ and $m_s$ sharply rise in contrast with $P_d(L/2, L/2)$, which vanishes. This coexistent state of SF and AF orders is realized by combining reformation of the bands [Fig. 4(b)] with a variation in spin.
correlation, particularly, AF correlation of the nearest-neighbor factor $\eta_0^2$ [Fig. 4(d)]. As a result, the sign of $E_{J(3)}$ is reversed and $E_{tot}$ is reduced, stabilizing the coexistent state. Although the regime of this exception is narrow and special, we take notice of it because the realized state has features of our interest. We take up two points:

(1) In this state, the orders of SF and AF coexist. In studies for the Hubbard model with $t'/t = 0$ [15], the AF order excludes the SF order and never coexists. This is interpreted as follows: The pure metallic AF state for $t'/t = 0$ is classified as type-I, which shows a pocket FS around the antinodal $\mathbf{k} = (\pi, 0)$ [7]. In contrast, the pure metallic SF state has a pocket FS around $\mathbf{k} = (\pi/2, \pi/2)$ in the nodal direction [4]. Therefore, the FS position of the subordinate

Figure 2. The total energy per site and its components, $E_{\alpha}/(N,t)$, are plotted as functions of doping rate $\delta$ for (a) $J^{(3)}/J = +1$, (b) $J^{(3)}/J = 0$, and (c) $J^{(3)}/J = -1$. Here, $E_{\alpha} = \langle \Psi | \hat{H}_\alpha | \Psi \rangle / \langle \Psi | \Psi \rangle$ with $\alpha = \text{tot}, t, t', J, J^{(3)}$ as in Eq. (1). Symbols indicate raw VMC data for $L = 12$, and straight dashed lines connecting both ends of each $E_{\text{tot}}$ curve are drawn as a guide to the eye.

Figure 3. The expectation values of the order parameters, namely, $P_d(\mathbf{r})$ (circles) for dSC, $|J_c|/t$ (inverted triangles) for SF, and $m_s$ (upward triangles) for AF, are plotted as functions of $\delta$ for (a) $J^{(3)}/J = +1$, (b) $J^{(3)}/J = 0$, and (c) $J^{(3)}/J = -1$. For (a) $J^{(3)}/J = +1$, $|J_c|/t$ is reduced, stabilizing the coexistent state. Although the regime of this exception is narrow and special, we take notice of it because the realized state has features of our interest. We take up two points:

(1) In this state, the orders of SF and AF coexist. In studies for the Hubbard model with $t'/t = 0$ [15], the AF order excludes the SF order and never coexists. This is interpreted as follows: The pure metallic AF state for $t'/t = 0$ is classified as type-I, which shows a pocket FS around the antinodal $\mathbf{k} = (\pi, 0)$ [7]. In contrast, the pure metallic SF state has a pocket FS around $\mathbf{k} = (\pi/2, \pi/2)$ in the nodal direction [4]. Therefore, the FS position of the subordinate
SF state is incompatible with that of the predominant AF state. On the other hand in the present case of $t'/t = -0.3$, the pure metallic AF state is classified as type-II [7], which has a pocket FS around $k = (\pi/2, \pi/2)$ in accordance with the SF state. The FS’s in the two states probably overlap with each other, resulting in the coexistence of SF and type-II AF orders.

(2) As seen in Fig. 4(a), small Pomeranchuk instability or nematicity— asymmetry between $x$ and $y$ directions—appears in this coexistent state, in contrast with the SC state. It is already known that Pomeranchuk instability vanishes in the $d$SC state [16, 17] but appears in the AF state up to $|1 - t_{1y}^{AF}/t_{1x}^{AF}| \sim 0.1$ [18]. We have confirmed that this instability remains $|1 - t_{1y}^{SF}/t_{1x}^{SF}| \sim 0.02$ for $\delta < 0.17$ in metastable pure SF states found (not shown). Thus, the 4-fold rotational symmetry is subtly broken in the optimized SF state. If the SF state gives a sizable contribution to the pseudogap phase in finite temperatures, this symmetry breaking will be observed.

4. Summary
We have studied the coexistence or exclusivity of the SF and $d$SC orders in the $t$-$t'$-$J$ model on the bases of VMC calculations. Using a mixed state which can simultaneously represent both orders, we found that, in almost all cases, the SF order is excluded in the more stable $d$SC state, and the two orders never coexist. This feature is consistent with that in the Hubbard model.
An exception is found for $J^{(3)}/J = -1$ near half filling, in which the optimized state has finite SF and AF orders but no dSC order. By analyzing this state, two interesting facts are found: (1) type-II AF and SF orders coexist, and (2) Pomeranchuk instability appears in the SF state, similarly to the AF state. Detailed description will be given elsewhere.

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