Interplay between staggered flux and $d$-wave superconducting states in Hubbard 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 the strong candidate for the pseudogap state. To this end, we use a variational Monte Carlo method for the square Hubbard model with diagonal transfer $t'$. In the trial wave function, $d$SC and SF orders coexist, which allows a continuous description of their interplay; essential factors for Mott physics and band renormalization are also included. It is found that the SF state does not coexist with $d$SC and is unstable for $U/t = 12$ regardless of the value of $t'/t$ within the present work.

1. Introduction

In understanding superconductivity (SC) in high-$T_c$ cuprates, what is the origin of pseudogap phenomena, which behave like a shadow of SC, is a long-standing problem [1, 2]. Among various candidates for the pseudogap state proposed so far, a staggered flux (SF) state was found to be moderately stable and have properties consistent with the behaviors in the pseudogap phase of cuprates, using a variational Monte Carlo (VMC) method for the square Hubbard model with diagonal transfer $t'$ [3]. In this study, it is shown that the SF state becomes more stable than the normal state (projected Fermi sea) for a strongly correlated and underdoped area by introducing a configuration-dependent phase factor, which is vital to treat a current-carrying state for a large $U/t$ [4], although the $d_{x^2-y^2}$-wave SC ($d$SC) state always has lower energy. 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 to that of $d$SC, especially, for $t'/t = -0.3$ [3]. Meanwhile, some experiments reported coexistence of the pseudogap and $d$SC gaps [5].

Thus, it is important to check directly whether the SF and $d$SC orders coexist or are mutually exclusive, because the SF and $d$SC states have been independently treated so far. In the present study, we will directly check this problem using a mixed state of the SF and $d$SC orders. We apply a VMC method to the Hubbard ($t$-$t'$-$U$) model on a square lattice with the fixed value of $U/t = 12$, and for $t'/t = 0$ and $-0.3$ for comparison, to cope with strong correlations. In the trial wave function, we introduce the following features:

(i) We allow for the coexistence of SF and $d$SC orders, by which we can treat a continuous description of their interplay.
(ii) The configuration-dependent phase-adjusting factor, vital in SF state for a large $U/t$ [3, 4], is introduced in addition to the ordinary Gutzwiller correlation [6] and refined doublon-holon (D-H) binding factors, which are crucial to describe Mott physics [7, 8, 9, 10].

(iii) The band renormalization effect is considered by adjusting the parameters of hopping integrals up to the fifth-neighbor sites; this effect is crucial near half filling [11, 12, 13].

On the basis of the data for optimized states, we find that the SF order competes with the $d$SC order and is not stabilized.

2. Method
We consider the Hubbard model on a square lattice with the next-nearest-neighbor transfer $t'$, shown in Fig. 1 (a),

\[
\mathcal{H} = \mathcal{H}_t + \mathcal{H}_U = -t \sum_{\langle rr' \rangle, \sigma} (c^\dagger_{r,\sigma} c_{r',\sigma} + \text{h.c.}) - t' \sum_{\langle rr' \rangle, \sigma} (c^\dagger_{r,\sigma} c_{r',\sigma} + \text{h.c.}) + U \sum_n n_{r \uparrow} n_{r \downarrow},
\]

where $c^\dagger_{r,\sigma}$ creates an electron of spin $\sigma$ at site $r$, $n_{r \sigma} = c^\dagger_{r,\sigma} c_{r,\sigma}$, and $\langle rr' \rangle$ and $\langle rr' \rangle$ denote indices of nearest-neighbor and diagonal-neighbor pairs, respectively. In the following, we use the square lattice of $N_s (= L \times L)$ sites with periodic-antiperiodic boundary conditions, and the unit of distance is the lattice constant.

As a variational wave function, we use a Jastrow type, $\Psi = \mathcal{P} \Phi$, where $\mathcal{P}$ is a many-body correlation factor as introduced below. For the one-body part $\Phi$, we adopt a coexisting 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 [14, 15, 16],

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

\[ \varphi_k = \frac{\Delta(k)}{\epsilon_{\text{SC}}(k) - \zeta + \sqrt{(\epsilon_{\text{SC}}(k) - \zeta)^2 + \Delta(k)^2}}, \]  

with \( \Delta(k) = \Delta_0(\cos k_x - \cos k_y) \). \( \alpha_{\lambda, k, \sigma}^\dagger \) in Eq. (2) is a creation operator of a quasi-particle in SF state that is constructed by diagonalizing a SF Hamiltonian \( \mathcal{H}^{\text{SF}}(\theta) \) as follows. The noninteracting SF Hamiltonian in the sublattice (A,B) representation, shown in Fig. 1 (b), is written as [3],

\[ \mathcal{H}^{\text{SF}} = -t \sum_{r \in A, \sigma} \left[ e^{i\theta} a_{r, \sigma}^{\dagger} (b_{r+x, \sigma} + b_{r-x, \sigma}) + e^{-i\theta} a_{r, \sigma}^{\dagger} (b_{r+y, \sigma} + b_{r-y, \sigma}) + \text{h.c.} \right]. \]  

Here, \( a_{r, \sigma}^{\dagger} (b_{r, \sigma}) \) creates an electron with spin \( \sigma \) on a sublattice A (B), and \( x \) (\( y \)) is the unit vector in the \( x \) (\( y \)) direction [\( x = (1, 0) \), \( y = (0, 1) \)].

By applying a Bogoliubov transformation,

\[ a_{k, \sigma} = \frac{\Gamma(k, \theta)}{\sqrt{2}} (\alpha_{-, k, \sigma} - \alpha_{+, k, \sigma}), \quad b_{k, \sigma} = \frac{1}{\sqrt{2}} (\alpha_{-, k, \sigma} + \alpha_{+, k, \sigma}), \]  

with

\[ \Gamma(k, \theta) = \frac{u(k, \theta)}{S(k, \theta)}, \]  

\[ u(k, \theta) = e^{i\theta} \cos k_x + e^{-i\theta} \cos k_y, \]  

\[ S(k, \theta) = \sqrt{u(k, \theta) u^*(k, \theta)} = \sqrt{\cos^2 k_x + 2 \cos(2\theta) \cos k_x \cos k_y + \cos^2 k_y}, \]

and \( a_{k, \sigma} (b_{k, \sigma}) \) being a Fourier transformation of \( a_{r, \sigma} (b_{r, \sigma}) \), \( \mathcal{H}^{\text{SF}} \) in Eq. (4) is diagonalized as

\[ \mathcal{H}^{\text{SF}} = \sum_{k, \sigma} \sum_{\lambda = \pm} \epsilon_{\lambda}^{\text{SF}}(k, \theta) \alpha_{\lambda, k, \sigma}^{\dagger} \alpha_{\lambda, k, \sigma}, \]

where the upper and lower band dispersions are given by

\[ \epsilon_{\pm}^{\text{SF}}(k, \theta) = \pm 2t S(k, \theta). \]  

Corresponding creation operators of the quasi-particle for the upper and lower band, which constitute Cooper pairs in Eq. (2), are obtained by the inverse transformation of Eq. (5) as

\[ \alpha_{\pm.k, \sigma}^{\dagger} = \frac{1}{\sqrt{2}} \left( \mp \Gamma(k, \theta) a_{k, \sigma}^{\dagger} + b_{k, \sigma}^{\dagger} \right), \]

where the phase \( \theta \), which is introduced into Eq. (2) through \( \alpha_{\lambda, k, \sigma}^{\dagger} \), is a variational parameter to be optimized together with the other parameters.

In addition, band renormalization effect owing to electron correlation is introduced. To this end, we assume that \( \epsilon_{\text{SC}}^{\text{SF}}(k) \) in Eq. (3) is fitted by a tight-binding band composed of transfers up to fifth-neighbor sites as shown in Fig. 2,

\[ \epsilon_{\text{SC}}^{\text{SF}}(k) = -2(t_{1x} \cos k_x + t_{1y} \cos k_y) - 4t_2 \cos k_x \cos k_y - 2t_3 [\cos(2k_x) + \cos(2k_y)] - 4t_4 [\cos(2k_x) \cos(k_y) + \cos(k_x) \cos(2k_y)] - 2t_5 [\cos(3k_x) + \cos(3k_y)]. \]
where \( t_{1y} \) and \( t_{2-5} \) are variational parameters to be optimized and \( t_{1x}/t \) is fixed to 1. In Eq. (12), asymmetry in \( t_1 \) is also introduced between \( x \) and \( y \) directions (\( t_{1x} \) and \( t_{1y} \)) to deal with the Pomeranchuk instability [11, 12].

For the Jastrow correlation factor \( \mathcal{P} \) in \( \Psi \), we assume the form \( \mathcal{P} = \mathcal{P}_\phi \mathcal{P}_Q \mathcal{P}_G \), where \( \mathcal{P}_G \) is a usual on-site (Gutzwiller) projection [6], \( \mathcal{P}_G = \prod_r (1-\Delta(r^\uparrow n_{r^\downarrow} n_{r^\downarrow})) \), and \( \mathcal{P}_Q \) is an extended projection between a doubly occupied site (doublon, D) and an empty site (holon, H), which controls the probability weight of D-H binding classified by the surrounded configuration, namely, the number of H neighboring D and vice versa [9, 10].

\( \mathcal{P}_\phi \) is a configuration-dependent phase-adjusting factor that partially cancels out the phase \( \theta \) in the processes of creating or annihilating D-H pairs [3, 4]:

\[
\mathcal{P}_\phi = \exp \left[ i\phi \sum_r \lambda_{AB}(r) \left( -h_{r+x} - h_{r-x} + h_{r+y} + h_{r-y} \right) \right],
\]

(13)

where \( d_r = n_{r^\uparrow} n_{r^\downarrow} \), \( h_r = (1-n_{r^\uparrow})(1-n_{r^\downarrow}) \), and \( \lambda_{AB}(r) = +1(-1) \) if \( r \in \text{A(B) lattice} \). The value of \( \phi \) is determined variationally. \( \mathcal{P}_\phi \) plays a vital role in the strongly correlated regime because a hopping process of annihilating a D-H pair such as \(|\uparrow, 0\rangle \rightarrow |\uparrow, \downarrow\rangle \) does not necessarily occur immediately after a D-H pair creating process, in which extra phase \( \theta \) is added, and then \( \theta \) should be canceled in each hopping process. Unless \( \mathcal{P}_\phi \) is introduced, the energy of the SF state does not decrease at all from that of the normal state [3].

In \( \Phi \), variational parameters to be optimized are \( \Delta_d, \zeta, \theta, t_{1y} \) and \( t_{2-5} \). Besides these eight in \( \Phi \), variational parameters in the correlation factor \( \mathcal{P} \) are \( g \) in \( \mathcal{P}_G, \phi \) in \( \mathcal{P}_\phi \), and 20 parameters in \( \mathcal{P}_Q \). According to a standard procedure of VMC, we obtain the optimal set of the 30 parameters by minimizing the energy. Using the optimized wave functions, we calculate various quantities. In particular, we take notice of the order parameters of dSC and SF orders in this work. The real-space dSC correlation function for the nearest-neighbor pairing is defined by

\[
P_d(r) = \frac{1}{N_s} \sum_{r'} \sum_{\tau, \tau'} \lambda_{xy}(\tau) \lambda_{xy}(\tau') \langle \Delta(\tau' + r, \tau) \Delta(\tau', \tau') \rangle,
\]

(14)

with

\[
\Delta(\tau, \tau') = \frac{1}{\sqrt{2}} (c_{r^\uparrow} c_{r^\uparrow + \tau^\downarrow} - c_{r^\downarrow} c_{r^\downarrow + \tau^\downarrow}),
\]

\( \lambda_{xy}(\tau) = +1 \) for \( \tau = (\pm 1, 0) \), and \( \lambda_{xy}(\tau) = -1 \) for \( \tau = (0, \pm 1) \). We use \( P_d(r) \) at the farthestmost distance \( r = (L/2, L/2) \) as a measure of dSC order. As the order parameter of the SF phase, we calculate a circular current defined as

\[
J_C/t = \frac{1}{N_s} \sum_{r \in A, \sigma} \sum_{\tau} \lambda_{xy}(\tau) \text{Im} \langle c_{r^\uparrow + \tau^\downarrow, \sigma}^\dagger c_{r, \sigma} - c_{r^\downarrow, \sigma}^\dagger c_{r^\uparrow + \tau^\downarrow, \sigma} \rangle.
\]

(15)
As pilot calculations, we have fixed the value of $U/t$ at 12 as a typical case of strongly correlated regime, and compare the results of $t'/t = 0$ and $t'/t = -0.30$ for systems of $L = 10$ and $L = 12$.

3. Results and discussion

To begin with, let us look at the optimized values of variational parameters in $\Psi$. In Fig. 3, the optimized values of the relevant variational parameters, the pairing gap $\Delta_d$ for $d$SC and two phases $\theta$ and $\phi$ for SF, are plotted as a function of doping rate $\delta$ for (a) $t'/t = 0$ and (b) $t'/t = -0.30$. For all range within the present calculations, $\Delta_d$ has finite values but both phases of SF state vanish, meaning that a SF order is absent and a pure $d$SC is realized.

![Figure 3](image)

Figure 3. Optimized values of relevant variational parameters in $\Psi$, the pairing gap $\Delta_d$ and SF phases $\theta$ and $\phi$, are plotted as a function of doping rate $\delta$ for (a) $t'/t = 0$ and (b) $t'/t = -0.30$.

Corresponding to these optimized parameters, the expectation values of order parameters estimated by the optimized $\Psi$ show the same tendency as seen in Fig. 4: the circular current of SF $j_{c}$ scarcely flows, whereas the pair correlation function $P_d(L/2, L/2)$ has finite values for all range within the present calculations. This indicates that the pure $d$SC is realized, whose properties are described in detail in Refs.[13, 17].

From these results, SF and $d$SC states are mutually exclusive and SF is unstable in a wide range of $\delta$ for strongly correlated Hubbard model. In Ref.[3], we argued that the reason why $d$SC and SF orders do not coexist is that the SF state has no Fermi surface around the antinodes $(\pm \pi, 0), (0, \pm \pi)$, which is necessary to induce $d$SC. However, now we deduce from the behavior of different mixed states [18] that the above explanation might be incorrect. The problem of compatibility and exclusivity of the two orders in a mixed state can be considered as follows.

First, we define the predominant (subordinate) state in a mixed state as its pure state has a lower (higher) energy than the pure state of the other. (i) The order of the predominant state necessarily arises, if its pure state exhibits an order at a given model parameter. (ii) If the resultant electronic state is (in)compatible with the subordinate state, the two orders are coexistent (the pure state with the predominant order appears without subordinate order).

In the present case, the $d$SC (SF) state is predominant (subordinate). Therefore, a more appropriate explanation for the exclusive feature is that when $d$SC is realized, the Fermi surface along $(\pi, 0)-(0, \pi)$ is smeared out by the $d$SC gap except for the point in the nodal direction. This is incompatible with the claim that the SF state has a pocket Fermi surface along $(\pi, 0)-(0, \pi)$. 


Figure 4. The order parameters of the two states are compared, which are obtained using the optimized $\Psi$. Namely, $d$-wave nearest-neighbor pair correlation function $P_d(r)$ for farthest distance $r = (L/2, L/2)$ (triangles) and circular current of SF $|J_c|/t$ (circles) as a function of $\delta$ for (a) $t'/t = 0$ and (b) $t'/t = -0.30$.

4. Summary
We have studied the interplay between SF and dSC in strongly correlated Hubbard model, using a coexisting wave function of SF and dSC orders in VMC calculations. These VMC results claim that the SF state is unstable and does not coexist with dSC for all range within the present calculations. It will be intriguing to search for interplay between SF and other orders because the properties of the SF state are mostly consistent with the behaviors in the pseudogap phase of cuprates as discussed in Ref.[3]. These are left for future studies.

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