Possibility of Pomeranchuk instability in staggered flux state

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Abstract. In connection with the symmetry-breaking phenomena found in cuprate superconductors, the instability toward $x$-$y$ and $(x+y)$-$(-x-y)$ anisotropy (Pomeranchuk instability) is studied for a strongly correlated Hubbard model ($U/t=12$) on a square lattice with the next-nearest-neighbor transfer $t'$ using a variational Monte Carlo method. As a variational function, a staggered flux state $\Psi_{SF}$ is considered, which is a candidate for the pseudogap state in cuprates. $\Psi_{SF}$ is stabilized in a underdoped regime and reduced to the normal state (projected Fermi sea) for larger doping area. By analyzing $\Psi_{SF}$ for $t'/t=0, \pm 0.3$, we argue that the appearance of Pomeranchuk instability is limited to the normal state with $t'/t=0$ and $0.08 \lesssim \delta \lesssim 0.20$ ($\delta$: doping rate) in the $x$-$y$ anisotropy. Band-renormalization effects (Fermi-surface modification) owing to strong correlations play a crucial role for the argument.

1. Introduction
Recently, symmetry-breaking phenomena have been successively found in cuprate superconductors; electronic nematic orders breaking the rotational symmetries \cite{1, 2} and charge density wave (CDW) breaking the translational symmetry \cite{3} were experimentally discovered along with superconductivity (SC) below the pseudogap temperature. A possible origin of the nematicity in cuprates is the Pomeranchuk instability (PI) that breaks four-fold rotational symmetry of the Fermi surface (FS) without lattice distortion \cite{4, 5, 6, 7, 8}.

In the preceding study \cite{9}, we discussed whether PI spontaneously occurs in the two-dimensional strongly correlated Hubbard model, using a variational Monte Carlo (VMC) method. There, we analyzed three trial states, namely, $\Psi_{SC}$ for $d_{x^2-y^2}$-wave SC, $\Psi_{AF}$ as an antiferromagnetic (AF) state, and $\Psi_{N}$ as a normal (paramagnetic) metallic state. For judging PI, we calculated an anisotropy indicator $A_{\ell}$ for the $\ell$-th neighbor hoppings, defined by

\[
A_{1} = |h(1,0) + h(-1,0) - h(0,1) - h(0,-1)|,
A_{2} = |h(1,1) + h(-1,-1) - h(1,-1) - h(-1,1)|,\tag{1}
\]

where

\[
h(\tau_{\ell}) = \frac{1}{N_{s}} \sum_{r,\sigma} \langle c_{r,\sigma}^\dagger c_{r+\tau_{\ell},\sigma} + \text{h.c.} \rangle\tag{2}
\]
is the expectation value of bare electron-hoppings, and \( \mathbf{\tau}_I \) is a vector connecting neighbor sites; \( \mathbf{\tau}_1 = \pm(1, 0), \pm(0, 1) \) for the nearest-neighbors, or \( \mathbf{\tau}_2 = \pm(1, 1), \pm(1, -1) \) for the second-nearest-neighbors. For \( A_I \sim 0 \), hoppings are isotropic, whereas for appreciable finite values of \( A_I \), hoppings become anisotropic between the orthogonal directions. For finite system sizes of \( N_s (= L \times L) \), \( A_I \) is sensitive to the existence of electrons that occupy k-points in the reciprocal space asymmetrically (asymmetric electrons) on FS and such anisotropy irregularly appears with respect to doping rate \( \delta \). This makes it complicated to determine whether or not the anisotropy remains in the thermodynamic limit. On the contrary, however, taking advantage of this anisotropy for finite \( L \), we empirically found criteria to judge the appearance of PI for finite \( U/t \) as follows [9]:

(A) At least, a part of the asymmetric electrons on FS for noninteracting case \( (U/t = 0) \) varies the k-point positions by a band-renormalization effect (BRE) owing to electron correlation when \( U/t \) is introduced. The asymmetric electrons that change the position necessarily move so as to increase the magnitude of momentum in a direction (say \(|k_y|\)) and decrease the magnitude of momentum in the counter direction (say \(|k_x|\)).

(B) Such behavior continuously appears for a finite range of \( \delta \) for any \( L \) (for excluding the specificity in system sizes).

Using the anisotropy indicators and criteria above, we argued that a tendency toward PI is limited to the normal state of a narrow range of the model parameters [9]. This result is reinforced by adding new data of \( L = 14 \), as shown in Fig. 1 for example: For the normal state, irregular behavior of \( A_I \) with respect to \( \delta \) is caused by a finite-size effect, namely, \( (x+y)-(x-y) \) anisotropy is not existent or negligible if any. On the other hand, \( A_I \) for \( \Psi_{\text{AF}} \) continuously exhibits finite values for \( 0.05 \lesssim \delta \lesssim 0.20 \) regardless of \( L \), meaning that the \( x-y \) anisotropy probably remains in the limit of \( L \rightarrow \infty \). In the robust ordered states \( (\Psi_{\text{SC}}, \Psi_{\text{AF}}) \), a tendency toward \( x-y \) and \( (x+y)-(x-y) \) anisotropy is suppressed because the isotropic (quasi-) FS’s

![Figure 1](image-url)

**Figure 1.** \( \delta \) dependence of anisotropy indicator \( A_1 \) \((x−y)\) and \( A_2 \) \([x+y]−(x−y)\) for the three state: \( \Psi_N \) (Normal) [first row, (a)–(c)], \( \Psi_{\text{SC}} \) (pure SC) [second row, (d)–(f)], and \( \Psi_{\text{AF}} \) (pure AF) [third row, (g)–(i)]. From left to right, the system size \( L \times L \) is increased: \( L = 10, 12, \) and \( 14 \). In all panels, \( t'/t = 0 \) and \( U/t = 12 \).
suited to the orders have priority; the irregular anisotropy appearing in $A_\ell$ for $\Psi_{AF}$ is no more than a subordinate to the nested FS necessary to the robust AF order. The SC ordered state exhibits good isotropy, as shown in Figs. 1 (d)–(f): SC is realized by the electron scattering of $Q = (\pi, \pi)$ that connects the antinodal areas. Therefore, it needs underlying FS near the antinodal points, which compete with PI. We consider that PI for ordered states is very weak, if any. Thus, the appearance of PI is limited to the normal state with $t'/t = 0$ and $0.05 \lesssim \delta \lesssim 0.20$ in the $x$–$y$ anisotropy.

In the present article, we address the same problem for a staggered flux (SF) state, which is one of the likely candidates for the pseudogap state proposed so far: a SF state was shown to be moderately stable and have properties consistent with the behaviors in the pseudogap phase of cuprates, using a VMC method for the square Hubbard model [10]. On the basis of these previous results, we study the feature of the SF state with an emphasis on anisotropy. It is found that the SF state is stable against PI like the AF or SC ordered state, and only the normal state is susceptible to the $x$–$y$ anisotropy in a narrow range of the model parameters.

2. Method

We consider the Hubbard model on a square lattice with the next-nearest-neighbor transfer $t'$,

$$\mathcal{H} = -t \sum_{(rr')_\sigma} \left( c_{r,\sigma}^\dagger c_{r',\sigma} + \text{h.c.} \right) - t' \sum_{(rr')_\sigma} \left( c_{r,\sigma}^\dagger c_{r',\sigma} + \text{h.c.} \right) + U \sum_r n_{r^+} n_{r^-},$$

where $c_{r,\sigma}$ creates an electron of spin $\sigma$ at site $r$, $n_{r^+} = c_{r,\sigma}^\dagger c_{r,\sigma}$, and $\langle rr' \rangle$ and $(rr')$ denote indices of nearest-neighbor and next-nearest-neighbor pairs, respectively. Here, the model with negative (positive) $t'/t$ corresponds to a hole-doped (electron-doped) cuprate for less-than-half-filled electron densities ($n = 1 - \delta < 1$). In the following, we use the square lattice of $L \times L$ sites with periodic-antiperiodic (P-AP) boundary conditions, and the unit of distance is the lattice constant.

As a variational wave function, we use a Jastrow type, $\Psi_{SF} = \mathcal{P} \Phi_{SF}$, where $\mathcal{P}$ is a many-body correlation factor as introduced below. For the one-body part, we adopt a pure SF state

![Figure 2](image_url)

**Figure 2.** (a) Schematic figure of the staggered flux state. Arrows denote the local circular current, which flows in an alternate direction in each plaquette. (b) Definition of hopping integrals $t_\ell$ as band parameters. They are classified by intersite distance and optimized variationally.
\[ \Phi_{SF} = \prod_{\{k\}_{occ}} \alpha_{k,\sigma}^\dagger |0\rangle, \]
where \(\{k\}_{occ}\) indicates the set of occupied points of wave-number vector \(k\), and \(\alpha_{k,\sigma}^\dagger\) is a creation operator of a quasi-particle in the SF state that is constructed by diagonalizing a SF Hamiltonian \(H_{SF}\) as follows [11, 12].

We introduce BRE into \(\Phi_{SF}\) by extending the hopping integrals up to fifth-neighbor sites, which are optimized variationally. The noninteracting SF Hamiltonian with transfers up to the fifth-neighbor sites in the sublattice (A, B) representation, shown in Fig. 2 (a), is written as,

\[ H_{SF}(\theta) = \sum_{k,\sigma} \left( \alpha_{k,\sigma}^\dagger b_{k,\sigma}^\dagger \right) \left( \begin{array}{cc} \varepsilon_{2}^{SF}(k) + \varepsilon_{3}^{SF}(k) & u(k, \theta) \\ u^*(k, \theta) & \varepsilon_{2}^{SF}(k) + \varepsilon_{3}^{SF}(k) \end{array} \right) \left( \begin{array}{c} a_{k,\sigma} \\ b_{k,\sigma} \end{array} \right), \tag{4} \]
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),

\[ u(k, \theta) = -2t_{1x} e^{i\theta} \cos k_x - 2t_{1y} e^{-i\theta} \cos k_y + \varepsilon_{4}^{SF}(k) + \varepsilon_{5}^{SF}(k), \tag{5} \]
and

\[ \begin{align*}
\varepsilon_{2}^{SF}(k) &= -2t_{2x} \cos(k_x - k_y) - 2t_{2y} \cos(k_x + k_y) \\
\varepsilon_{3}^{SF}(k) &= -2t_{3} [\cos(2k_x) + \cos(2k_y)] \\
\varepsilon_{4}^{SF}(k) &= -4t_{4} [\cos(2k_x) \cos(k_y) + \cos(k_x) \cos(2k_y)] \\
\varepsilon_{5}^{SF}(k) &= -2t_{5} [\cos(3k_x) + \cos(3k_y)].
\end{align*} \quad \tag{6} \]
To consider PI, we introduce asymmetries in \(t_1\) between \(x\) and \(y\) (lattice) directions and \(t_2\) between \(x' = x - y\) and \(y' = x + y\) (diagonal) directions, as shown in Fig. 2 (b). Here, \(t_{1x}\) is fixed at \(t\) in Eq. (3) for normalization, and other hopping integrals \((t_{1y}, t_{2x'}, t_{2y'}, t_{3-5})\) are variational parameters. Note that the phase \(\theta\) is accompanied by only the nearest-neighbor transfer \(t_1\) but not by \(t_2\) - \(t_5\) here.

By applying a Bogoliubov transformation,

\[ a_{k,\sigma} = \frac{\Gamma(k, \theta)}{\sqrt{2}} (-\alpha_{k,\sigma} + \beta_{k,\sigma}), \quad b_{k,\sigma} = \frac{1}{\sqrt{2}} (\alpha_{k,\sigma} + \beta_{k,\sigma}) \tag{7} \]
with

\[ \Gamma(k, \theta) = \frac{u(k, \theta)}{S(k, \theta)}, \quad S(k, \theta) = \sqrt{u(k, \theta) u^*(k, \theta)} \tag{8} \]
\(H_{SF}(\theta)\) in Eq. (4) is diagonalized as

\[ H_{SF}(\theta) = \sum_{k,\sigma} \left( \varepsilon_{\pm}^{SF}(k, \theta) \alpha_{k,\sigma}^\dagger \alpha_{k,\sigma} + \varepsilon_{\pm}^{SF}(k, \theta) \beta_{k,\sigma}^\dagger \beta_{k,\sigma} \right) \tag{9} \]
where the lower and upper band dispersions are given by

\[ \varepsilon_{\pm}^{SF}(k, \theta) = \pm S(k, \theta) + \varepsilon_{2}^{SF}(k) + \varepsilon_{3}^{SF}(k). \tag{10} \]

Corresponding creation operators of the quasi-particle for the lower and upper band are obtained by the inverse transformation of Eq. (7) as

\[ \alpha_{k,\sigma}^\dagger = \frac{1}{\sqrt{2}} (-\Gamma(k, \theta) a_{k,\sigma}^\dagger + b_{k,\sigma}^\dagger), \quad \beta_{k,\sigma}^\dagger = \frac{1}{\sqrt{2}} (+\Gamma(k, \theta) a_{k,\sigma}^\dagger + b_{k,\sigma}^\dagger) \tag{11} \]
respectively, where the phase \( \theta \), which is introduced into \( \Psi_{\text{SF}} \) through \( \alpha_{k,\sigma}^\dagger \), is a variational parameter to be optimized together with the other parameters.

For the Jastrow correlation factor \( P \) in \( \Psi_{\text{SF}} \), we assume the form \( P = P_\phi P_Q P_G \), where \( P_G \) is a usual on-site (Gutzwiller) projection \([13]\), \( P_G = \prod_r [1 - (1 - g) n_r \sigma n_r \sigma] \), and \( P_Q \) 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 \([14, 15]\).

\( P_\phi \) is a configuration-dependent phase-adjusting factor that partially cancels out the processes in the creation or annihilating D-H pairs \([10, 16]\):

\[
P_\phi = \exp \left[ i \phi \sum_r \lambda_{AB}(r) \ d_r (-e_{r+x} - e_{r-x} + e_{r+y} + e_{r-y}) \right],
\]

where \( d_r = n_r \sigma n_r \sigma, \ e_r = (1 - n_r \uparrow)(1 - n_r \downarrow) \), \( x \) (\( y \)) is the unit vector in the \( x \) (\( y \)) direction \((x = (1, 0), y = (0, 1))\), and \( \lambda_{AB}(r) = +1(-1) \) if \( r \in A(B) \) lattice. The value of \( \phi \) is determined variationally. \( P_\phi \) plays a vital role in treating a current-carrying state for large \( U/t \).

In \( \Psi_{\text{SF}} \), variational parameters to be optimized are \( \theta, t_{1y}, t_{2y'}, t_{2y''}, t_3 \). Besides these seven in \( \Psi_{\text{SF}} \), variational parameters in the correlation factor \( P \) are \( g \) in \( P_G \), \( \phi \) in \( P_\phi \), and 10 parameters in \( P_Q \). According to a standard procedure of VMC, we obtain the optimal set of the 19 parameters by minimizing the energy. When SF state approaches normal state (\( \theta \to 0 \)) for large \( \delta \), the variational energy for finite \( L \) becomes flat and discontinuous as a function of the band parameters. In this case, we cannot use general optimization methods based on the derivatives of energy \([17]\). Instead, we repeat the following procedures several times: (1) We find an approximate minimum on the mesh of \( t_{1y}, t_{2y'}, t_{2y''} \), and \( t_3 \) with the other parameters fixed. (2) We optimize the other variational parameters by a standard procedure.

Using the optimized wave functions, we calculate a circular current as the order parameter of the SF phase:

\[
J_c/t = \frac{1}{N_s} \sum_{r \in A, \sigma} \sum_{\tau_1} \lambda_{xy}(\tau_1) \text{Im}(c_{r+\tau_1, \sigma}^\dagger c_{r, \sigma} c_{r, \sigma}^\dagger c_{r+\tau_1, \sigma}),
\]

where \( \tau_1 = (\pm 1, 0), (0, \pm 1) \). The anisotropy is checked by anisotropy indicators in Eq. (1) and also by contour maps of the momentum distribution function, \( n(k) = (1/2) \sum_\sigma (c_{k, \sigma}^\dagger c_{k, \sigma}) \).

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 \( t'/t = \pm 0.3 \) for systems of \( L = 10 \) and \( L = 12 \).

3. Results and discussions

Before discussing anisotropy, we survey some relevant feature of \( \Psi_{\text{SF}} \) briefly. In Fig. 3, \( \delta \) dependence of the order parameter for SF is shown. For \( t'/t = 0 \) and \( t'/t = +0.3 \), the stable SF area with finite \( |J_c|/t \) is limited to the narrow range in a low doping regime \( (\delta < 0.08) \), and SF state is reduced to the normal state (\( \theta \sim 0 \) and \( \phi \sim 0 \)) for larger \( \delta \). This stable SF area expands to \( \delta \lesssim 0.16 \) for \( t'/t = -0.3 \). These results are in good agreement with those of Ref. \([10]\).

This stability of \( \Psi_{\text{SF}} \) for \( t'/t = -0.3 \) originates primarily from the large \( t'/t \) dependence of \( \Psi_N \) and the small \( t'/t \) dependence of \( \Psi_{\text{SF}} \) \([10]\). For example, \( \Psi_N \) has the maximum energy at \( t'/t \sim -0.3 \) for \( \delta \sim 0.08 \), while the energy of \( \Psi_{\text{SF}} \) is almost flat with respect to \( t'/t \) because the nature of \( \Psi_{\text{SF}} \), appropriately defined for \( t'/t = 0 \), is basically unchanged for \( t'/t \neq 0 \) \([17]\). As a result, \( \Psi_{\text{SF}} \) is relatively stabilized and the stable SF area expands for \( t'/t = -0.3 \).

Next, we consider the anisotropy in the normal state with \( |J_c|/t \sim 0 \) in Fig. 3 \( (\delta \gtrsim 0.08 \ (0.16) \ for \ t'/t = 0, +0.3 \ (-0.3)) \). Shown in Fig. 4 is the \( \delta \) dependence of the anisotropy indicators \( A_\ell \)
to the normal state in the range of larger $A$. Electrons move by BRE. The red bold points indicate the occupied $k$-points in Fig. 5. We show typical PI is restricted to the area of $0 < L < 10$. Criteria are satisfied in this case. To summarize the normal state, the possibility of appearing $k$-magnitude of momenta in $U/t$ for $U/t = 0$. As will be discussed for $t'/t = 0$, we consider that $(x + y) - (x - y)$ anisotropy is not existent or negligible if any. On the other hand, $A_1$ for $t'/t = 0$ is added with a broken line in (a).

$\text{Figure 3.}$ The expectation values of the order parameter for SF, $|J_c|/t$, are plotted as functions of $\delta$ for (a) $t'/t = -0.3$, (b) $t'/t = 0$, and (c) $t'/t = +0.3$. Data for $L = 10$ and 12 are simultaneously plotted.

$\text{Figure 4.}$ $\delta$ dependence of anisotropy indicator $A_1$ $(x-y)$ and $A_2$ $[(x + y) - (x - y)]$ estimated by the optimized $\Psi_{SF}$ for $L = 12$. The value of $t'/t$ increases from left to right, $t'/t = -0.3$, 0, and +0.3. For a detailed analysis for $t'/t = -0.3$, $A_1$ for $L = 10$ is added with a broken line in (a).

$[\text{Eq. (1)}]$. $A_2$ irregularly becomes anisotropic ($A_2 \neq 0$) with respect to $\delta$ and we confirmed that there is no case that simultaneously satisfies the criteria (A) and (B) mentioned above. Thus, we consider that $(x + y) - (x - y)$ anisotropy is not existent or negligible if any. On the other hand, $A_1$ for $t'/t = 0$ is appreciably large both for $L = 10$ and 12. Therefore, as to the criterion (A), we carefully check that a systematic transition of $k$-points on FS appears, as will be discussed for $t'/t = 0$ (Fig. 5). As for $t'/t = \pm 0.3$, we cannot find it for every $\delta$ and $L$. Thus, we judge that the normal state for $t'/t = \pm 0.3$ is stable against PI.

As for $t'/t = 0$, $A_1$ continuously has large values for $0.08 \lesssim \delta \lesssim 0.20$ as seen in Fig. 4 (b). In Fig. 5, we show typical $k$-point configurations in this range of $\delta$, to verify how asymmetric electrons move by BRE. The red bold points indicate the occupied $k$-points in $\Psi_{SF}$ with BRE for $U/t = 12$, while the blue open circles indicate those in the simple Fermi sea without BRE for $U/t = 0$. We find, in every panel, electrons with maximum magnitude of momentum in $k_x$ direction for $U/t = 0$ (blue circles without red dots) move to the $k$-points of the maximum magnitude of momenta in $k_y$ direction (red dots without blue circles). This confirms that the criteria are satisfied in this case. To summarize the normal state, the possibility of appearing PI is restricted to the area of $0.08 \lesssim \delta \lesssim 0.20$ for $t'/t = 0$.

Now, we move to PI in the stable SF that has finite value of $|J_c|/t$ in Fig. 3. As seen in Fig. 4, $A_1$ for the SF state irregularly becomes nonzero but seems suppressed as a whole as compared to the normal state in the range of larger $\delta$, where $\Psi_{SF}$ is reduced to $\Psi_N$. Here, we carry out an
analysis of $k$-point occupation and confirmed that no case simultaneously satisfies the criteria. Thus, the SF state is considered stable against PI. This also can be read from $n(k)$ shown in

Figure 5. Comparison of occupied $k$-points between noninteracting ($U/t = 0$, blue open circles) and strongly correlated ($U/t = 12$, red bold dots) cases for $t'/t = 0$. We select the data from the area in $\delta$ of possible PI ($0.08 \lesssim \delta \lesssim 0.20$).

Figure 6. Contour maps of the momentum distribution function $n(k)$ for $t'/t = 0$ and $L = 12$. Data for $\delta = 0.083$–0.139 are compared between the stable SF state with finite $|J_c|/t$ [first row, (a)–(c)] and normal state with $|J_c|/t \sim 0$ [second row (d)–(f)]. The thick pink line in each panel indicates a (quasi-) Fermi-level line obtained by connecting the points of $(1 - \delta)/2$. 

Fig. 6. In contrast with the normal state with $|J_x|/t \sim 0$, in which the $x$-$y$ anisotropy manifests itself, the SF state exhibits better isotropy except for expected anisotropy owing to the P-AP boundary condition used here. The reason can be explained as follows: Because the SF state has a pocket FS around $(\pi/2, \pi/2)$ in the nodal direction [10, 18], asymmetric electrons tend to exist near the $(\pi/2, \pi/2)$ in a low doping regime. If asymmetric electrons exist near $(\pi/2, \pi/2)$, $(x+y)-(x-y)$ anisotropy tends to be enhanced. Such a feature of SF order is actually seen in the behavior of $A_\ell$. Thus, the anisotropy appearing in $A_\ell$ is no more than an artifact caused by the specificity of finite-size effect and will disappear in the thermodynamic limit. We consider that PI in SF state is very weak, if any.

4. Summary
We discussed the possibility of arising PI in a SF state for a strongly correlated Hubbard model on the basis of VMC calculations. For the stable SF ordered state, appearing in the underdoped regime, a tendency toward $x$-$y$ or $(x+y)-(x-y)$ anisotropy is suppressed because the isotropic (quasi-) Fermi surfaces suited to the SF orders have priority. The possibility of arising PI is limited to the normal state of a specific range of doping rate and $t'/t$. Analyses of other possible symmetry-breaking phenomena such as CDW, incommensurate AF, and the extended $s+d$-wave SC are left for future studies.

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[18] In the contour maps in Figs. 6(b) and 6(c), the pocket FS's are not clear because the magnitude of pocket FS's are small for small $\delta$ and the k-point resolution is coarse owing to finite system sizes (See, for instance, Fig.13(b) in Ref.[10]). However, the contours in Figs. 6(b) and 6(c) are concave near $(\pi/2, \pi/2)$, which suggests the existence of pocket FS's. Such concavity cannot be seen in the other densities.