Mott Transitions and Staggered Orders in the Three-component Fermionic System: Variational Cluster Approach

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The variational cluster approximation is used to study the ground-state properties and single-particle spectra of the three-component fermionic Hubbard model defined on the two-dimensional square lattice at half filling. First, we show that either a paired Mott state or color-selective Mott state is realized in the paramagnetic system, depending on the anisotropy in the interaction strengths, except around the SU(3) symmetric point, where a paramagnetic metallic state is maintained. Then, by introducing Weiss fields to observe spontaneous symmetry breakings, we show that either a color-density-wave state or color-selective antiferromagnetic state is realized depending on the interaction anisotropy and that the first-order phase transition between these two states occurs at the SU(3) point. We moreover show that these staggered orders originate from the gain in potential energy (or Slater mechanism) near the SU(3) point but originate from the gain in kinetic energy (or Mott mechanism) when the interaction anisotropy is strong. The staggered orders near the SU(3) point disappear when the next-nearest-neighbor hopping parameters are introduced, indicating that these orders are fragile, protected only by the Fermi surface nesting.

1. Introduction

The many-particle physics of multicomponent fermions in correlated electron systems, such as orbital orderings,1) orbital-selective Mott transitions,2) and orbital-spin liquids,3) has recently been one of the major themes of condensed matter physics. The ground-state properties of the N-component model with N > 2, where N is the number of internal degrees of freedom of a fermion, are conjectured to depend strongly on N, and therefore the occurrence of novel quantum phases at N > 2 has been anticipated.4) In particular, the SU(N) symmetric model has been of great interest for simulating systems of correlated fermionic ultracold atoms in optical lattices.5−9) Thus, the possible experimental realization of systems with N > 2 will provide a good opportunity in the research field of quantum many-body problems, of which the candidates may be the SU(6) symmetry for 173Yb,10,11) the SU(6)×SU(2) symmetry for a mixture of 171Yb and 173Yb,12) the SU(10) symmetry for 87Sr,13,14) and a three-component fermionic system, although not exactly SU(3), for 6Li.15,16)

The three-component fermionic Hubbard model, which is a natural extension of the two-component one for correlated electrons, has recently been studied to clarify its metal-insulator transition, translational-symmetry-broken staggered orders, and superfluidity. Namely, dynamical mean field theory (DMFT) calculations have shown that the metal-insulator transition in the paramagnetic state of the N = 3 Hubbard model at half filling (or 3/2 fermions per site) does not occur at the SU(3) symmetric point but it occurs when the interaction strengths between components are anisotropic.17−19) Moreover, the DMFT calculations assuming translational symmetry breaking have shown that two types of staggered orders appear, depending on the anisotropy in the interaction strengths, and the first-order phase transition occurs between the two at the SU(3) symmetric point.19−22) Superfluidity has also been reported to occur, even in the repulsive Hubbard model near half filling, when the interaction strengths are anisotropic, suggesting the presence of an exotic pairing mechanism,19,23−25) where the fluctuations of the staggered orders may cause the pairing. We may therefore point out that the effects of the lattice geometry and Fermi surface nesting, which are important in the formation of the staggered orders, should be examined carefully in the low-dimensional systems.

In this paper, motivated by the above developments in the field, we study the ground-state properties and excitation spectra of the three-component fermionic Hubbard model defined on the two-dimensional square lattice at half filling by means of the variational cluster approximation (VCA). The VCA can treat the short-range spatial correlations precisely in the thermodynamic limit of low-dimensional systems and therefore has a major advantage that the effects of the lattice geometry and Fermi surface topology can be examined, which DMFT studies cannot tackle. We thereby hope that some new insights into the physics of three-component fermionic systems will be obtained.

First, we calculate the single-particle spectrum, density of states, and single-particle gap in the paramagnetic state to study the Mott transitions of the model, and we draw its ground-state phase diagram, which includes three distinct Mott phases. Then, we introduce the Weiss fields to study the translational symmetry breakings and show that two types of staggered orders appear in the ground state of the model. We moreover examine the origin of the long-range orderings in terms of the gains in kinetic and potential energies, addressing the Slater versus Mott mechanisms. We also examine the stability of the staggered orders by introducing the next-nearest-
neighbor hopping parameters to destroy the Fermi surface
nesting. We thereby discuss the characteristic properties
of the three-component fermionic system defined
on the two-dimensional square lattice.

This paper is organized as follows. In Sect. 2, we in-
troduce the three-component Hubbard model and briefly
summarize the method of VCA. In Sect. 3, we present
calculated results for the paramagnetic and staggered or-
dered states and give some discussion. A summary of the
paper is given in Sect. 4.

2. Model and Method

2.1 Three-component Hubbard model

The three-component Hubbard model may be defined by
the Hamiltonian

\[
\mathcal{H} = -t \sum_{\langle i,j \rangle} \sum_{\alpha} c_{i\alpha}^\dagger c_{j\alpha} - \sum_{i} \sum_{\alpha} \mu_{\alpha} n_{i\alpha}
+ \frac{1}{2} \sum_{i} \sum_{\alpha \neq \beta} U_{\alpha\beta} n_{i\alpha} n_{i\beta},
\]

(1)

where \( c_{i\alpha}^\dagger \) \( (c_{i\alpha}) \) denotes the creation (annihilation) op-
erator of a fermion with color \( \alpha \) \( (=a,b,c) \) at site \( i \) and
\( n_{i\alpha} = c_{i\alpha}^\dagger c_{i\alpha} \). \( t \) is the hopping integral between the neigh-
boring sites, which is taken as the unit of energy, and \( U_{\alpha\beta} \)
\( (=U_{\beta\alpha}) \) is the on-site interaction between two fermions
with colors \( \alpha \) and \( \beta \). Throughout the paper, we assume
the color-dependent interactions and set \( U_{ab} = U \) \( (>0) \)
and \( U_{bc} = U_{ca} = U' \) \( (>0) \) for simplicity. We also assume
the filling of \( n = \sum_{i} n_{i\alpha} = 3/2 \) \( (\text{denoted as half filling}) \),
where \( n_{i\alpha} \equiv \sum_{n,\alpha}(n_{i\alpha})/L = 1/2 \) is the average
number of color-\( \alpha \) fermions in a system of size \( L \). We set the
chemical potential as \( \mu_{\alpha} = \sum_{\beta \neq \alpha} U_{\alpha\beta}/2 \)
to maintain the average particle density at \( n = 3/2 \).

This model with \( U = U' \) corresponds to the SU(3) Hubbard
model, using which studies have been carried out on superfluidity in the presence of attractive
interactions as well as on the metal-insulator transition in the presence of repulsive interactions.\(^{26-31}\) In particular, it has been confirmed\(^{11} \) that this model at half filling does not show the Mott transition in the paramagnetic state, maintaining the metallic state irrespective of the interaction strength, unlike in the two-component Hubbard model. At \( U' = 0 \), on the other hand, the two interacting components undergo the Mott transition, leaving the noninteracting component metallic. Thus, the anisotropy in the interaction strengths \( (U \neq U') \) causes the Mott transition: at \( U \gg U' \), the color-selective Mott (CSM) state is realized, where the two components are localized and one component is itinerant, and at \( U \ll U' \), the paired Mott (PM) state is realized, where the two components are paired in the same sites and one component is localized in the other sites.\(^ {18,19,24}\)

In the presence of long-range staggered orders, it is known that fermions are arranged alternately in the lattice and either the color-selective antiferromagnetic (CSAF) state corresponding to the CSM state at \( U \gg U' \) or the color-density-wave (CDW) state corresponding to the PM state at \( U \ll U' \) is realized.\(^ {19,21}\) It has been pointed out\(^ {19} \) that in the SU(3) symmetric \( U = U' \) Hubbard model, the CDW state is realized at half filling if the perfect Fermi surface nesting of the nesting vector \( Q = (\pi, \pi) \) exists in the two-dimensional square lattice. It has also been pointed out\(^ {19,20} \) that in the SU(3) symmetric model at half filling, the CSAF and CDW states are energetically degenerate at zero temperature and that the CSAF state is realized at \( U > U' \) and the CDW state is realized at \( U < U' \). DMFT calculations have suggested the presence of an \( s^- \)-wave superfluid state at \( U' > U > 0 \), which is, however, higher in energy than the CDW state and is not realized as the ground state of the system.\(^ {21,24} \)

2.2 Variational cluster approximation

To accomplish the calculations in the thermodynamic limit, we use the VCA\(^ {32,33} \) based on self-energy functional theory (SFT), which is the variational principle for the grand potential as a functional of the self-energy.\(^ {33-35} \) Unlike in DMFT, we can thereby precisely take into account the effects of short-range spatial fermionic correlations in low-dimensional systems. In fact, successful explanations were given for the antiferromagnetism and superconductivity,\(^ {36} \) as well as for the pseudogap behaviors,\(^ {37} \) in the two-dimensional Hubbard model for high-\( T_c \) cuprate materials. The trial self-energy for the variational method is generated from the exact self-energy of the disconnected finite-size clusters, which act as a reference system. To investigate the spontaneous symmetry breaking in the VCA,\(^ {38} \) we introduce the Weiss fields in the system as variational parameters. The Weiss fields of the CDW and CSAF states are defined as

\[
\mathcal{H}'_{\text{CDW}} = M'_{\text{CDW}} \sum_{i} e^{iQ \cdot r_{i}} (n_{ia} + n_{ib} - n_{ic})
\]

(2)

\[
\mathcal{H}'_{\text{CSAF}} = M'_{\text{CSAF}} \sum_{i} e^{iQ \cdot r_{i}} (n_{ia} - n_{ib}) ,
\]

(3)

respectively, where \( M'_{\text{CDW}} \) and \( M'_{\text{CSAF}} \) are the strengths of the Weiss fields of the CDW and CSAF states, respectively, which are taken as the variational parameters. Then, the Hamiltonian of the reference system is given by \( \mathcal{H}' = \mathcal{H} + \mathcal{H}'_{\text{CDW}} + \mathcal{H}'_{\text{CSAF}} \). Within SFT, the grand potential at zero temperature is given by

\[
\Omega = \Omega' - \frac{1}{N_s} \oint_{C} \frac{dz}{2\pi i} \sum_{K,\alpha} \ln \text{det} \left[ I - V_{\alpha}(K) G'_{\alpha}(z) \right] , \quad (4)
\]

where \( \Omega' \) is the grand potential of the reference system, \( N_s \) is the number of clusters in the system, \( I \) is the unit matrix, \( V_{\alpha} \) is the hopping parameter between the adjacent clusters, and \( G'_{\alpha} \) is the exact Green’s function of the reference system calculated by the Lanczos exact-diagonalization method. The \( K \)-summation is performed in the reduced Brillouin zone of the superlattice and the contour \( C \) of the frequency integral encloses the negative real axis. The variational parameters are optimized on the basis of the variational principle, i.e., \( \partial \Omega/\partial M'_{\text{CDW}} = 0 \) for the CDW state and \( \partial \Omega/\partial M'_{\text{CSAF}} = 0 \) for the CSAF state. The solutions with \( M'_{\text{CDW}} \neq 0 \) and \( M'_{\text{CSAF}} \neq 0 \) correspond to the CDW and CSAF states, respectively. In our VCA calculations,
we assume the two-dimensional square lattice and the modulation vector is given by \( Q = (\pi, \pi) \). We use an \( L_c = 2 \times 3 \) site cluster as the reference system.

To calculate the single-particle spectrum and density of states (DOS), we use cluster perturbation theory (CPT), which proceeds by tiling the lattice into identical, finite-size clusters, solving many-body problems in these clusters exactly, and treating the intercluster hopping terms at the first order in strong-coupling perturbation theory. This theory is exact in both the strong and weak correlation limits, and provides a good approximation to the spectral function at any wave vector. In CPT, the Green’s function of color-\( \alpha \) fermions is given by

\[
G_{\alpha}^{\text{cpt}}(k, \omega) = \frac{1}{L_c} \sum_{i,j=1}^{L_c} G_{ij,\alpha}(k, \omega)e^{-ik(r_i-r_j)},
\]

where \( G_{\alpha}(k, \omega) = \left[ G_{\alpha}^{-1}(\omega) - V_\alpha(K) \right]^{-1} \). Using the CPT Green’s function \( G_{\alpha}^{\text{cpt}} \), the single-particle spectral function of the color-\( \alpha \) fermions is defined as

\[
A_{\alpha}(k, \omega) = -\frac{1}{\pi} \text{Im} \ G_{\alpha}^{\text{cpt}}(k, \omega + i\eta),
\]

where \( \eta \) gives the artificial Lorentzian broadening of the spectrum. We also calculate the DOS of the color-\( \alpha \) fermions defined as

\[
\rho_{\alpha}(\omega) = \frac{1}{L} \sum_k A_{\alpha}(k, \omega),
\]

where \( L = N_s L_c \) is the total number of lattice sites in the system.

### 3. Results of Calculations

#### 3.1 Mott transitions in the paramagnetic state

First, let us discuss the Mott metal-insulator transitions in the paramagnetic state (or in the absence of the Weiss fields). Using the CPT, we calculate the single-particle spectra and DOS, the results of which are shown in Fig. 1 as a function of \( U/t \) at \( U'/t = 4 \). At \( U/t = 0 \), where the PM state is realized [see Fig. 2(a)], we find that the gap opens in all components of the spectra at the Fermi level; in particular, the gap in the c component is about twice as large as the gap in the a and b components. This may be understood as follows: if a color a (or b) fermion is added to the system, it is placed on the site occupied by the color c fermion due to the Pauli principle, which increases the energy of the system by \( U' \), but if a color c fermion is added to the system, it is placed on the site occupied doubly by the color a and b fermions, which increases the energy of the system by \( 2U' \). Thus, a gap of size \( U' \) (\( 2U' \)) opens in the a and b components (c component) of the spectra.

With increasing \( U/t \), we find that the gap in the a and b components decreases and closes at a certain \( U/t \) value, but the gap in the c component remains open up to a larger \( U/t \) value. Then, at \( U/t = U'/t = 4 \), where our model is SU(3) symmetric, the spectra become equivalent in all the components and the system becomes metallic as shown in Fig. 1(g).

Increasing the \( U/t \) value further, we find that a gap opens again in the a and b components, but the c component remains metallic and the DOS curve resembles that of the noninteracting band in the two-dimensional square lattice. This situation occurs because the color a and b fermions are localized owing to the large \( U/t \) values, whereas the color c fermions hop freely because the interaction strengths are the same, \( U'_{bc} = U'_{ca} = U' \). In this CSM state, a gap of size \( U' \) opens in the a and b components of the spectra because, if a color a (b) fermion is added to the system, it is placed on the site occupied by the color b (a) fermion due to the Pauli principle, which increases the energy of the system by \( U' \).

Note that the size of the single-particle gap cannot be estimated accurately in Fig. 1 because the spectra are broadened artificially by \( \eta \) [see Eq. (6)]. However, the chemical-potential dependence of the average particle number per site \( n_\alpha \) enables us to evaluate the gap size accurately, which may be calculated as

\[
n_\alpha = \frac{1}{L} \sum_{i=1}^{L} \langle n_{i\alpha} \rangle = \frac{1}{N_s L_c} \int \frac{d\omega}{2\pi i} \sum_{K} \sum_{i=1}^{L_c} G_{i\alpha,\alpha}(K, \omega)
\]

via the diagonal term of the Green’s function \( G_{\alpha}^{\text{cpt}} \). The particle number \( n_\alpha \) calculated as a function of the chemical potential \( \mu_\alpha \) is fixed to \( n_\alpha = 0.5 \) at half filling if the system is metallic, but it shows a plateau in the range \( \mu_\alpha \leq U/t \), whereas the color c fermion is localized owing to the large \( U/t \) value. Then, at \( \mu_\alpha = 2U/t \), the gaps \( \Delta_a, \Delta_b \) in all components decreases and closes at a certain \( \mu_\alpha = U/t \), as shown in Figs. 1(g)-1(i).

The sizes of the gaps are \( U' \) in the a and b components and \( 2U' \) in the c component, as we have discussed above, so that we obtain the relation \( \Delta_a \approx 2\Delta_b \). With increasing \( U/t \), the gaps \( \Delta_a \) decrease linearly, and in the region corresponding to Figs. 1(d)-1(f), we find the \( \Delta_a = \Delta_b = 0 \) and \( \Delta_c > 0 \), the region of which we call CSM(I), where the color a and b fermions have metallic behavior and the color c fermions have insulating behavior. Upon increasing \( U/t \) further, the gap in the c component also closes, and around \( U/t = U' \), the gaps in all the components close (\( \Delta_c = 0 \)), as shown in Figs. 1(g)-1(i).

In the large-\( U/t \) (\( \gg U'/t \)) region, we have \( \Delta_a = \Delta_b = 0 \) and \( \Delta_c = 0 \), the state of which we call CSM(I), where the gaps \( \Delta_c (\alpha = a, b) \) increase linearly with \( U \), indicating that the CSM(I) phase is caused by \( U \). The critical phase boundaries determined at \( U'/t = 4 \) are \( U/t \leq 1.8 \) for PM, \( 1.8 \leq U/t \leq 3.1 \) for CSM(I), and \( 5.1 \leq U/t \) for CSM(I).

Figure 2 shows the phase diagram determined by the thus calculated gaps \( \Delta_\alpha \), where we find three Mott phases, PM, CSM(I), and CSM(II), as well as the paramagnetic metallic phase. The CSM(I) phase appears at \( U \gg U' \) and the PM phase appears at \( U \ll U' \), whereas around the SU(3) symmetric point \( U = U' \), we find the...
paramagnetic metallic phase. The newly found CSM(II) phase appears between the PM and paramagnetic metallic phases, where only the color $c$ fermions are gapful. This phase appears because the single-particle excitation requires twice the energy for the $c$ component as for the $a$ and $b$ components, as shown above. This phase is absent in the DMFT calculations, suggesting its absence in the case of infinite dimensions; thus, we consider that the intersite spatial correlations between fermions in two-dimension, which the VCA takes into account properly, may induce this CSM(II) phase.

![Fig. 1.](image1.png) (Color online) Calculated DOSs and single-particle spectra in the normal state of our model [Eq. (1)]. The $U/t$ dependence at $U'/t = 4$ is shown, where the solid (dotted) lines indicate the results for the color $a$ and $b$ (color $c$) components. The dispersions of the spectra are shown along the line connecting the $\Gamma(0,0)$, $X(\pi,0)$, and $M(\pi,\pi)$ points of the Brillouin zone. The artificial Lorentzian broadening of the spectra $\eta/t = 0.1$ is used.

![Fig. 2.](image2.png) (Color online) Left panel: Calculated single-particle gap $\Delta_\alpha$ for color $\alpha$ fermions as a function of $U/t$ at $U'/t = 4$. Right panel: Calculated phase diagram of the paramagnetic state in the parameter space $(U/t,U'/t)$, which includes the paired Mott (PM) and two types of color-selective Mott (CSM) phases. Illustrated below are their schematic representations.

![Fig. 3.](image3.png) (Color online) Calculated ground-state energies $E_0/t$ (left panel) and staggered magnetizations $M_\alpha$ (right panel) of the color-density-wave (CDW) and color-selective antiferromagnetic (CSAF) states as a function of $U/t$ at $U'/t = 4$. Illustrated below are schematic representations of the CDW and CSAF states.

### 3.2 Staggered ordered states

Next, let us discuss the symmetry-broken staggered ordered states, which are obtained by adding the Weiss fields defined in Eqs. (2) and (3) to the Hamiltonian in Eq. (1). We thereby calculate the ground-state energy per site, $E_0 = \Omega + \sum_\alpha \mu_\alpha$, and the staggered magnetization of color $\alpha$ fermions defined as

$$M_\alpha = \frac{1}{L} \sum_i (\langle n_{i\alpha} \rangle - \langle n_{i\alpha} \rangle)_c e^{\mathbf{Q} \cdot \mathbf{r}_i}$$

for the optimized Weiss fields.

$$\frac{1}{N_s L_c} \frac{H_c}{\gamma t} \sum_{\mathbf{K}} \sum_{i=1}^{L_s} G_{i,k}(\mathbf{K},z) e^{\mathbf{Q} \cdot r_i}$$
The results are shown in Fig. 4, where we find that the spectral peak positions do not change markedly in comparison with those of the corresponding PM and CSM(I) phases, whereas sharp coherence peaks appear at the edges of the gap in both the CDW and CSAF phases. These gaps become wider than those of the corresponding PM and CSM(I) phases, reflecting the stabilization of the ordered phases.

3.3 Slater versus Mott mechanisms

In the previous subsection, we showed that the CDW and CSAF phases are stabilized for $U < U'$ and $U > U'$, respectively, and that the first-order phase transition occurs between the two phases at $U = U'$. If we assume the paramagnetic phase, the Mott insulating phases such as PM and CSM are stabilized when the interaction strengths are strongly anisotropic (see Fig. 2), but the paramagnetic metallic phase is maintained around the SU(3) symmetric point ($U = 0$). These gaps become wider than those of the corresponding CDW and CSAF phases, indicating that either the CDW or CSAF phase can appear. The calculated staggered magnetization indicates that $M'_\text{CDW} \neq 0$ at $U > U'$, where the CDW state is stable. In particular, we find that $M_a = M_b > 0$ and $M_c < 0$, which indicate that the color $a$ and $b$ fermions are located on the same sites and the color $c$ fermions are located alternately on other sites, resulting in the staggered order of the modulation vector $Q = (\pi, \pi)$. At $U > U'$, we find that $M'_\text{CSAF} \neq 0$, where the CSAF state is stable. In particular, we find that $M_a > 0, M_b < 0$, and $M_c = 0$, which indicate that the color $a$ and $b$ fermions show staggered antiferromagnetic orderings but the color $c$ fermions do not.

We also calculate the single-particle spectra and DOSs for the staggered ordered CDW and CSAF phases, where we use the optimized Weiss fields $M'_{\text{CDW}}$ and $M'_{\text{CSAF}}$. The results are shown in Fig. 4, where we find that the spectral peak positions do not change markedly in comparison with those of the corresponding PM and CSM(I) phases, whereas sharp coherence peaks appear at the edges of the gap in both the CDW and CSAF phases.
It is known that there are two mechanisms for the stabilization of staggered orders.\(^\text{42-44}\) One is the Slater mechanism, which occurs in itinerant systems, where the Fermi surface instability causes band folding and gap opening due to the interactions between fermions, leading to staggered orderings in the system, resulting in gains in the potential energy but losses in the kinetic energy. The other is the Mott mechanism, which occurs in insulating systems, where the virtual hopping of fermions aligns their colors antiferromagnetically due to the Pauli principle, leading to staggered orderings in the system, resulting in gains in the kinetic energy but losses in the potential energy. Below, we calculate the kinetic and potential energies in the paramagnetic and staggered ordered phases of the system, and consider the mechanisms of the staggered orderings from the energetic point of view.

Let us define the potential \(E_{U,ab}\) and kinetic \(E_{K,a}\) energies per site as

\[
E_{U,ab} = \frac{1}{L} \sum_i \langle n_{a \alpha} n_{b \beta} \rangle = U_{a \beta} \frac{\partial E_0}{\partial U_{a \beta}} \tag{10}
\]

\[
E_{K,a} = \frac{1}{L} \left( \sum_{i,j} \left( \epsilon^+_{a \alpha} c_{j \alpha} \right) \right) = -\frac{\partial E_0}{\partial n_{a \alpha}} \tag{11}
\]

and their energy gains caused by the staggered orderings as

\[
\Delta E_{U,ab}^{\text{DW}} = E_{U,ab}^{\text{DW}} - E_{U,ab}^{\text{N}} \tag{12}
\]

\[
\Delta E_{K,a}^{\text{DW}} = E_{K,a}^{\text{DW}} - E_{K,a}^{\text{N}} \tag{13}
\]

for the CDW phase at \(U \leq U'\), and as

\[
\Delta E_{U,ab}^{\text{AF}} = E_{U,ab}^{\text{AF}} - E_{U,ab}^{\text{N}} \tag{14}
\]

\[
\Delta E_{K,a}^{\text{AF}} = E_{K,a}^{\text{AF}} - E_{K,a}^{\text{N}} \tag{15}
\]

for the CSAF phase at \(U > U'\), where the superscripts DW, AF, and N stand for the CDW, CSAF, and paramagnetic normal phases, respectively. Thus, comparing the signs and magnitudes of \(\Delta E_{U,ab}\) and \(\Delta E_{K,a}\), we can evaluate the energy gains in the formation of the staggered long-range order.

Figure 5 displays the calculated results for the quantities defined above as a function of \(U/t\) (\(U'/t\)) at a fixed value of \(U'/t\) (\(U/t\)). The same results along the line \(U/t = U'/t\) are also shown in Fig. 6. First, in Figs. 5(a)-5(c), where a comparison is made between the CDW and normal phases, we find that

\[
\Delta E_{U,ab}^{\text{DW}} + \Delta E_{U,ab}^{\text{AF}} < 0 \tag{16}
\]

\[
\Delta E_{K,a}^{\text{DW}} + \Delta E_{K,a}^{\text{AF}} > 0 \tag{17}
\]

\[
\Delta E_{K,a}^{\text{AF}} > 0 \tag{18}
\]

for \(0.0 \leq U'/t \leq 2.0\) at \(U/t = 0\), indicating that the gain in potential energy leads to the staggered CDW order. For \(4.0 \leq U'/t \leq 8.0\), however, the signs are inverted and we find that

\[
\Delta E_{U,ab}^{\text{DW}} + \Delta E_{U,ab}^{\text{AF}} > 0 \tag{19}
\]

\[
\Delta E_{K,a}^{\text{DW}} + \Delta E_{K,a}^{\text{AF}} < 0 \tag{20}
\]

\[
\Delta E_{K,a}^{\text{AF}} < 0, \tag{21}
\]

which indicates that the gain in kinetic energy leads to the staggered order. Thus, the stabilization mechanism of the CDW phase shows a crossover from the Slater mechanism to the Mott mechanism. With increasing \(U/t\), the interaction between the \(a\) and \(b\) components increases and \(\Delta E_{U,ab}^{\text{DW}}\) varies considerably as shown in Figs. 5(b) and 5(c). We then find that \(\Delta E_{U,ab}^{\text{DW}} > 0\) at \(U < U'\) and \(\Delta E_{U,ab}^{\text{DW}} < 0\) at \(U' \gg U\). We also find that around \(U = U'\), although the loss in the potential energy is large, \(\Delta E_{U,ab}^{\text{DW}} > 0\), the effect of \(\Delta E_{U,ab}^{\text{DW}} + \Delta E_{U,ab}^{\text{AF}} < 0\) is still dominant, leading to the Slater mechanism of the CDW ordering. This mechanism even occurs at large \(U = U'\) values [see Fig. 6(a)], suggesting that the effects of Fermi surface nesting are important here.

Next, in Figs. 5(d)-5(f) where a comparison is made between the CSAF and normal phases, we find that

\[
\Delta E_{U,ab}^{\text{AF}} < 0 \tag{22}
\]

\[
\Delta E_{K,a}^{\text{AF}} + \Delta E_{K,a}^{\text{AF}} > 0 \tag{23}
\]

for \(0.0 \leq U/t < 3.0\) at \(U'/t = 0\), indicating that the gain in potential energy leads to the staggered CSAF order. For \(3.5 \leq U/t \leq 8.0\), however, the signs are inverted and we find that

\[
\Delta E_{U,ab}^{\text{AF}} > 0 \tag{24}
\]

\[
\Delta E_{K,a}^{\text{AF}} + \Delta E_{K,a}^{\text{AF}} < 0, \tag{25}
\]

which indicates that the gain in kinetic energy leads to the staggered CSAF order. Thus, the stabilization mechanism of the CSAF phase also shows a crossover from the Slater mechanism to the Mott mechanism. With increasing \(U'/t\), the \(c\)-component-related quantities \(\Delta E_{U,ca}^{\text{AF}} + \Delta E_{U,ca}^{\text{AF}}\) and \(\Delta E_{K,c}^{\text{AF}}\) vary considerably as shown in Figs. 5(e) and 5(f). We then find that \(\Delta E_{U,ab}^{\text{AF}} + \Delta E_{U,ab}^{\text{AF}} > 0\) and \(\Delta E_{K,a}^{\text{AF}} < 0\) at \(U' \simeq U\), indicating that the \(c\)-component-related quantity loses its potential energy. However, we find that the \(a\)- and \(b\)-component-related quantity \(\Delta E_{U,ab}^{\text{AF}} < 0\) gains considerable potential energy, leading to the Slater mechanism of the CSAF ordering. At \(U' \gg U'\), on the other hand, we find that the gain in the kinetic energy of the \(a\)- and \(b\)-components is dominant, \(\Delta E_{K,a}^{\text{AF}} + \Delta E_{K,b}^{\text{AF}} < 0\), leading to the Mott mecha-
nism of the CSAF ordering. Note that the point where the signs of $\Delta E_{\alpha}^{AF}$ and $\Delta E_{\alpha}^{AF}$ are inverted approaches $U = U'$ with increasing $U'/t$, but the Slater mechanism of the CSAF stabilization even occurs at large $U = U'$ values [see Fig. 6(b)], suggesting that the effects of Fermi surface nesting are important around the SU(3) symmetric point, as in the case of the CDW stabilization.

We thus find that the Slater mechanism (Mott mechanism) of the staggered ordering predominantly occurs in the strong coupling region around the SU(3) symmetric point, as in the case of the CDW stabilization. Here, we confirm this expectation by introducing the next-nearest-neighbor hopping term to the Hamiltonian and destroying the Fermi surface nesting. The Fermi surface of the CDW stabilization even occurs at large $U = U'$. We also examined the kinetic and potential energy gains in the staggered orderings and showed that the Slater mechanism with a predominant potential energy gain occurs in the region around $U = U'$, where the metallic state is realized in the paramagnetic phase, and that the Mott mechanism with a predominant kinetic energy gain occurs in the region where the interactions are highly anisotropic and the Mott insulating state is realized in the paramagnetic phase.

By introducing the next-nearest-neighbor hopping parameters, we demonstrated that the Fermi surface nesting is essential in the region around $U = U'$, where the Slater mechanism occurs for the staggered orderings. This result indicates that the staggered orders near the SU(3) symmetric point are fragile, protected only by the Fermi surface nesting. A recent DMFT calculation has suggested that the $s$-wave superfluid state occurs as a metastable state at $U < U'$ in the three-component Hub-

![Fig. 7. (Color online) Left panel: Calculated order parameter of the CDW phase $M_a$ in the presence of the next-nearest-neighbor hopping $t'$. The $U/t$ dependence is shown at $U' = 4$. Right panel: Noninteracting Fermi surfaces at $t'/t = 0$ and $0.2$. The nesting vector at $t'/t = 0$ is indicated by arrows.](image)

3.4 Effects of Fermi surface nesting

Finally, let us discuss the effects of Fermi surface nesting on the staggered orders. In the previous subsection, we showed that the Slater mechanism for the stabilization of the staggered orderings occurs in the region of the isotropic interaction strengths around the SU(3) symmetric point, where we may expect that Fermi surface nesting plays an essential role in the formation of the staggered orders. Here, we confirm this expectation by introducing the next-nearest-neighbor hopping term to the Hamiltonian and destroying the Fermi surface nesting of $Q = (\pi, \pi)$. The Hamiltonian then reads

$$
\mathcal{H} = -t \sum_{\langle i,j \rangle} \sum_{\alpha} \epsilon_\alpha^i c_{\alpha i}^\dagger c_{\alpha j} - t' \sum_{\langle\langle i,j \rangle\rangle} \sum_{\alpha} \epsilon_\alpha^i c_{\alpha i}^\dagger c_{\alpha j,\alpha}
$$

$$
- \sum_{\alpha} \mu_\alpha n_{\alpha} + \frac{1}{2} U \sum_{\alpha \neq \beta} n_{\alpha} n_{\beta},
$$

where $t'$ is the next-nearest-neighbor hopping parameter and $\langle\langle i,j \rangle\rangle$ indicates the summation over the next-nearest-neighbor pairs of sites. The Fermi surface of the noninteracting system at $t'/t = 0.2$ is shown in Fig. 7, where we confirm that the nesting feature is completely destroyed. We employ the VCA to calculate the CDW order, where the Hamiltonian of the reference system is given by $\mathcal{H}' = \mathcal{H} + \mathcal{H}_\text{on} + \mathcal{H}_\text{CDW}'$ with the on-site potential $\mathcal{H}_\text{on} = \sum_{i,\alpha} \epsilon'_\alpha n_{\alpha i}$. We optimize the grand potential $\Omega$ with respect to both $M'_\text{CDW}$ and $\epsilon'_\alpha$; the latter is necessary to keep the average particle number at $n_\alpha = 0.5$ because the particle-hole symmetry is broken in this system due to the introduction of the $t'$ term.\(^{45}\)

The calculated results for the order parameter $M_\alpha$ are shown in Fig. 7, where we find that the region with a nonvanishing parameter shrinks with increasing $t'/t$ and that the paramagnetic phase without the CDW order actually appears around $U = U'$. We thus demonstrate that, in the region of $U \approx U'$, the Fermi surface nesting of $Q = (\pi, \pi)$ plays an essential role in the formation of the staggered CDW order, which is not important when $U \ll U'$. The Slater mechanism thus has a contrasting effect to the Mott mechanism for the stabilization of the staggered orders.

4. Summary

We have investigated the ground-state properties and excitation spectra of the three-component fermionic Hubbard model defined on the two-dimensional square lattice at half filling. We used the VCA, which enables us to study the effects of the lattice geometry and Fermi surface topology in the low-dimensional systems in the thermodynamic limit, precisely taking into account spatial fermion correlations.

First, we presented the ground-state phase diagram of the paramagnetic state of the model, whose phases include the paired Mott (PM) phase at $U \ll U'$, the color-selective Mott (CSM) phase at $U > U'$, and the paramagnetic metallic phase between them. We also showed that the Mott transition does not occur in the SU(3) symmetric point $U = U'$ and that a different CSM phase appears between the PM and paramagnetic metallic phases, where the color $a$ and $b$ fermions are metallic and color $c$ fermions are localized.

Next, we introduced the Weiss fields to find the spontaneous symmetry-broken phases and found that the color-density-wave (CDW) and color-selective antiferromagnetic (CSAF) phases appear at $U < U'$ and $U > U'$, respectively, and that the energies of the two phases cross at $U = U'$. We also examined the kinetic and potential energy gains in the staggered orderings and showed that the Slater mechanism with a predominant potential energy gain occurs in the region around $U = U'$, where the metallic state is realized in the paramagnetic phase, and that the Mott mechanism with a predominant kinetic energy gain occurs in the region where the interactions are highly anisotropic and the Mott insulating state is realized in the paramagnetic phase.
bard model at half filling.\textsuperscript{24} We may therefore suggest that this superfluid state can be most stable if the Fermi surface nesting is destroyed to suppress the CDW order because the pairing of two fermions at $k$ and $-k$ for the superfluidity is not affected strongly by the Fermi surface nesting. The exotic pairing mechanism for superfluidity in multicomponent fermionic systems of $N > 2$ may be an intriguing issue for future studies.

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