Predominant Magnetic States in Hubbard Model on Anisotropic Triangular Lattices

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Using an optimization variational Monte Carlo method, we study the half-filled-band Hubbard model on anisotropic triangular lattices, as a continuation of the preceding study [J. Phys. Soc. Jpn. 75 (2006) 074707]. We introduce two new trial states: (i) A coexisting state of $(\tau, \pi)$-antiferromagnetic (AF) and a $d$-wave singlet gaps, in which we allow for a band renormalization effect, and (ii) a state with an AF order of $120^\circ$ spin structure. In both states, a first-order metal-to-insulator transition occurs at smaller $U/t$ than that of the pure $d$-wave state. In insulating regimes, magnetic orders always exist; an ordinary $(\pi, \pi)$-AF order survives up to $t'/t \sim 0.9$ ($U/t = 12$), and a $120^\circ$-AF order becomes dominant for $t'/t \gtrsim 0.9$. The regimes of the robust superconductor and of the nonmagnetic insulator the preceding study proposed give way to these magnetic domains.

I. INTRODUCTION

A series of $\kappa$-(BEDT-TTF)$_2$X [$\kappa$-ET salts] have intriguing properties specific to strongly-correlated systems; they often undergo unconventional superconductor (SC)-to-insulator transitions through the chemical substitution of X or under applied pressure, and have good two-dimensionality in conductivity with frustrated lattice structure. As a model of these compounds, the half-filled-band Hubbard model on anisotropic triangular lattices 1 (an extended square lattice with hopping integral $t$ in $x$ and $y$ directions, and $t'$ in one diagonal direction [1,1]) has been intensively studied: 2

$$\mathcal{H} = \sum_{k\sigma} \varepsilon_k c_{k\sigma}^\dagger c_{k\sigma} + U \sum_i n_{i \uparrow} n_{i \downarrow}, \quad (1)$$

where $\varepsilon_k = -2t(\cos k_x + \cos k_y) - 2t'\cos(k_x + k_y)$, and $U, t, t' > 0$. To clarify the properties of this model in the strongly-correlated region, $U/t \gg 1$, especially Mott transitions, reliable theoretical approaches are needed. To this end, the present authors recently applied to eq. (1) an optimization (or correlated) variational Monte Carlo (VMC) method, which can deal with SC and a Mott transition as a continuous function of $U/t$. Henceforth, we call this preceding study \cite{1} \cite{2}. In (I), we chiefly considered various properties of the $d_{x^2-y^2}$-wave singlet state, $\Psi^d_{Q^d}$, and constructed a ground-state phase diagram in the $t'-U$ plane, by considering its energy with that of the ordinary $(\pi, \pi)$-antiferromagnetic (AF) state, $\Psi_{Q^d}^{AF}$. Most of the results are consistent with the behavior of $\kappa$-ET salts, but the area of an $(\pi, \pi)$-AF insulator is unexpectedly limited ($t'/t \lesssim 0.4$), in considering the appearance of the AF order in e.g., $\kappa$-(ET)$_2$CuN(CN)$_2$Cl ($t'/t \sim 0.74$), as well as the vanishing point of the AF order expected in the $J$-$J'$ Heisenberg model ($t'/t \sim 0.8$) \cite{11}. As we pointed out in (I), this disagreement possibly stems from the fact that the $d$-wave singlet state and the AF state were treated separately; thereby, the former state does not include a seed of an AF long-range order, and the latter a band renormalization effect.

For $t' \sim t$, many theoretical studies \cite{4} \cite{5} \cite{6} \cite{7} \cite{8} for the Hubbard model have obtained results of dominant nonmagnetic insulating state, which are consistent with the insulating state found in $\kappa$-(ET)$_2$Cu$_2$(CN)$_3$ with $t'/t \sim 1.06$ [9]. Nonetheless, we should be also concerned about the AF order with 120-degree spin structure, which is considered to prevail in the isotropic case of the $J$-$J'$-Heisenberg model. [10] [11] Actually, a recent VMC study \cite{12} for a $t$-$J$-type model on the isotropic triangular lattice concluded that the $120^\circ$-AF ordered state is dominant in an unexpectedly wide range of doping rate. Thus, it is possible that the $120^\circ$-AF order is robust also in the Hubbard model with $t' \sim t$ and sufficiently small values of $U/t$ for the organics.

In this paper, as a continuation of (I), we introduce two trial states: (i) A state which includes $(\pi, \pi)$-AF and $d$-wave gaps simultaneously: \cite{13} \cite{14} and then a band (or Fermi-surface) renormalization effect owing to the electron correlation is taken into account. \cite{15} (ii) A state which exhibits the $120^\circ$-AF order. In addition to these functions, we newly consider SC states with pairing symmetries suitable for $t' > t$. Our main interest here is the competition among these states and those treated in (I). It is found that first-order metal-to-insulator transitions always occur at smaller values of $U/t$ than those for the pure $d$-wave state. In the insulating regime, the $(\pi, \pi)$-AF order remains up to $t'/t \sim 0.9$, owing to the band renormalization effect we considered in the coexisting state, and the $120^\circ$-AF order becomes predominant in the range of $t'/t \gtrsim 0.9$. Consequently, a magnetic order, namely the $(\pi, \pi)$-AF or $120^\circ$-AF order, always exists in the insulating regime, and a regime of a nonmagnetic insulator vanishes. In addition, a domain of dominant SC found in (I) disappears within the present results. The previous phase diagram is substantially modified.

In [III] we explain the trial wave functions used, and recapitulate the main points of (I) as a motivation of this study. In [IV] we represent the VMC results. In [V] we briefly summarize this study, and compare with experimental and other
II. Wave Functions

As usual, we use Jastrow-type trial wave functions: \( \Psi = \mathcal{P}\Phi \), in which \( \Phi \) denotes a one-body (Hartree-Fock) part expressed as a Slater determinant, and \( \mathcal{P} \) a many-body correlation factor. In II A we describe the correlation factor \( \mathcal{P} \). In II B we point out insufficient points in the wave functions used in (I), and introduce a coexisting state of the \((\pi, \pi)\)-AF and \(d\)-wave gaps in which the one-body band structure is modified by optimizing a hopping parameter \(t'\), as renormalization owing to electron correlation. In II C we formulate a state with an AF order of 120° spin structure, as another new trial state. In II D we briefly touch on the conditions of the VMC calculations.

A. Correlation factor

When one treats the Hubbard model on the basis of a variational method, it is crucial to introduce, in addition to the well-known Gutzwiller (onsite) factor \( \mathcal{P}_G \), \(^{17,18}\) site-site correlation factors \(^{19,20}\) into Jastrow-type wave functions. In particular, near half filling, the binding effect of a doubly-occupied site (doublon) to an empty site (holon) is indispensable to describe a Mott transition as well as various quantities appropriately. \(^{19}\) To this end, we have repeatedly studied \(^3,21,22,23\) a four-body factor formally written as

\[
\mathcal{P}_Q = \prod_i (1 - \mu Q_i^\dagger) (1 - \mu' Q_i'^\dagger),
\]

in which \(d_i = n_i n_i, e_i = (1 - n_i)(1 - n_i)\), and \(\tau (\tau')\) runs over all the adjacent sites in the bond directions of \(t' (t')\). In eq. (2), \(\mu (\mu')\) is a variational parameter which controls the binding strength between a doublon and a holon in the bond direction \(t (t')\). We have confirmed that \(\mathcal{P}_Q\) works effectively in the model, eq. (1).

B. Coexisting state of \(d\)-wave and AF gaps

Using \(\mathcal{P} = \mathcal{P}_Q \mathcal{P}_G\), we mainly studied, in (I), a \(d_{x^2-y^2}\)-wave singlet state: \(\Psi_Q^d = \mathcal{P}\Phi_d\), where \(\Phi_d\) is the BCS function with a \(d_{x^2-y^2}\)-wave gap:

\[
\Delta_k = \Delta_d (\cos k_x - \cos k_y).
\]

In \(\Psi_Q^d\), we allow for renormalization of the one-body band \(\varepsilon_k\) owing to electron correlation, by varying \(t' (\equiv t')\) in \(\Phi_d\) as a variational parameter, \(^{15}\) independently of \(t'\) fixed in the Hamiltonian eq. (1). In (I), we obtained the following results within \(\Psi_Q^d\). (i) A first-order Mott (conductor-to-nonmagnetic-insulator) transition takes place for arbitrary \(t'/t\) at \(U = U_c\) roughly of the bandwidth. This transition is induced by the binding (and unbinding) of a doublon (negatively charged) to a holon (positively charged), unlike the famous Brinkman-Rice transition. \(^{24}\) (ii) Robust \(d\)-wave SC appears in a restricted parameter range immediately below \(U_c\) and of weak frustration \((t'/t \lesssim 0.7)\). This SC is considered to be induced by a short-range \((\pi, \pi)\)-AF spin correlation, because whenever the superconducting (SC) correlation function is sizably enhanced, the spin structure factor \(S(q)\) has a sharp peak at the AF wave number, \(q = Q = (\pi, \pi)\). (iii) In the insulating regime, \(\Psi_Q^d\) exhibits a spin-gap behavior and does not have an \((\pi, \pi)\)-AF long-range order, although \(S(q)\) has a sharp peak at \(q = Q\), namely a short-range AF correlation considerably develops.

To consider the competition between \(\Psi_Q^d\) and a state with the \((\pi, \pi)\)-AF long-range order [see Fig. II(a)], which should prevail for small \(t'/t\), we also studied a projected AF state, \(\Psi_Q^{AF} = \mathcal{P}\Phi_{AF}\), where \(\Phi_{AF}\) is a mean-field-type \((\pi, \pi)\)-AF state. In \(\Psi_Q^{AF}\), we did not renormalize \(t'\), because the variational energy \(E\) to be minimized becomes a discrete function of \(t'/t\). We found that \(\Psi_Q^{AF}\) is restricted to a weakly frustrated regime, \(t'/t \lesssim 0.4\) (for \(U/t = 6\)), and this range tends to shrink as \(U/t\) increases. As noted in (I), the above results (iii) and (iv) are not consistent with various approximate results \(^{10}\) for the corresponding \(J'\) spin model, which predict that the \((\pi, \pi)\)-AF domain continues up to \(t'/t \sim 0.8\). To resolve this disagreement, a seed of the AF order should be introduced into \(\Psi_Q^d\), and the renormalization of \(\varepsilon_k\) owing to \(U\) into \(\Psi_Q^{AF}\).

In this paper, we study a wave function, \(\Psi_{Q0}^{co} = \mathcal{P}\Phi_{co}\), which meets the above requirements by merging \(\Psi_Q^d\) and \(\Psi_Q^{AF}\). In \(\Psi_{Q0}^{co}\), the \(d\)-wave gap and an AF order can coexist. \(^{13}\) The one-body part is written as

\[
\Phi_{co} = \left( \sum_k \varphi_k b_{k,1}^\dagger b_{-k,1} \right) N_c/2 |0\rangle,
\]

in which \(N_c\) is the electron number, and \(\varphi_k\) is the ratio of BCS coefficients:

\[
\varphi_k = \frac{\Delta_k}{\varepsilon_k},
\]

with

\[
\varepsilon_k = -2t(\cos k_x + \cos k_y) - 2t' \cos (k_x + k_y),
\]

and \(b^\dagger\) is a creation operator that diagonalizes the ordinary \((\pi, \pi)\)-AF Hartree-Fock Hamiltonian, and is given as

\[
\begin{align*}
\beta_{k,\sigma}\left( \alpha_{k,\sigma} \right) &= \alpha_{k,\sigma} e_k + \beta_{k,\sigma} e_{k+K,\sigma}, \\
\alpha_{k,\sigma} \left( \beta_{k,\sigma} \right) &= \frac{1}{2} \left( 1 - (+) \right) \frac{\gamma_k}{\sqrt{\gamma_k^2 + \Delta_{AF}^2}}.
\end{align*}
\]
with $\gamma_k = -2t(\cos k_x + \cos k_y)$ and $\varsigma = +(-)1$, according as $\sigma = \uparrow (\downarrow)$. In addition to the six parameters in $\Psi^d_Q$, namely, $g$ (Gutzwiller (onsite) parameter), $\mu$, $\mu'$, $\Delta_d$, $\zeta$ (chemical potential) and $\hat{P}$, $\Psi^{cQ}_q$ has the seventh parameter $\Delta_{AF}$, which controls the staggered spin field and is closely connected to the $(\pi, \pi)$-AF order parameter $m_{\lambda}$ (sublattice magnetization). Note that, in contrast to $\Delta_{AF}$, a finite optimized value of $\Delta_d$ does not necessarily mean that a SC gap opens, but an insulating spin gap. For $\Delta_{AF}$ ($\Delta_d \to 0$), $\Psi^{cQ}_Q$ is reduced to $\Psi^d_Q$ ($\Psi^F_Q$). Thus, we may regard $\Psi^{cQ}_Q$ as $\Psi^d_Q$ in which the $(\pi, \pi)$-AF long-range order parameter can arise, and also as $\Psi^F_Q$ into which a band renormalization effect is introduced through the $d$-wave gap.

### C. AF-ordered state with 120-degree spin structure

As discussed in [10], an AF-ordered state with 120° spin structure [see Fig. 1(b)] is plausible for the region of $t'/t \sim 1$. We introduce such a state, $\Psi_{120} = c\Psi_{120}$, for the Hubbard model eq. (11), and check its stability for finite values of $U/t$ and consistency with the results obtained for $U/t = \infty$. [10][11]

As the one-body part, $\Psi_{120}$, we use a Hartree-Fock ground state for the Hamiltonian eq. (11). As explained in Fig. 2, we consider six sublattices (A-F); the spin quantization axis of a sublattice is turned by 60 degrees from that of a neighboring sublattice. Using this scheme, the Hamiltonian eq. (11) is transformed to

\[
H = -\sum_\lambda \left[ t \sum_{i,j,\lambda \neq \lambda_j} (a^\dagger_{i,\lambda,\uparrow} a^\dagger_{i,\lambda,\downarrow}) R \left( \frac{\pi}{6} \right) \left( a_{j,\lambda+\uparrow} a_{j,\lambda+\downarrow} \right) + t' \sum_{i,j,\lambda \neq \lambda_j} (a^\dagger_{i,\lambda,\uparrow} a^\dagger_{i,\lambda,\downarrow}) R \left( \frac{\pi}{3} \right) \left( a_{j,\lambda+2\uparrow} a_{j,\lambda+2\downarrow} \right) \right] + \text{h.c.}
\]

\[+ U \sum_\lambda \sum_i n^T_{i\uparrow} n^T_{i\downarrow}, \tag{11} \]

where

\[
R(\theta) = \begin{pmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{pmatrix}, \tag{12} \]

$a^\dagger_{i,\sigma}$ is a creation operator in the sublattice representation, $n^T_{i\sigma} = a^\dagger_{i,\sigma} a_{i,\sigma}$, $\lambda = \text{A-F}$ is a sublattice index, $i_\lambda$ runs over all the sites on sublattice $\lambda$, and an angle (round) bracket in the summation indices in eq. (11) indicates a nearest(diagonal)-neighbor pair. We apply a Hartee-Fock decoupling to the interaction term in eq. (11),

\[
\sum_i U n^T_{i\uparrow} n^T_{i\downarrow} \sim \sum_i U \left( \langle n^T_{i\uparrow} \rangle n^T_{i\downarrow} + \langle n^T_{i\downarrow} \rangle n^T_{i\uparrow} \right) + \text{const.}, \tag{13} \]

and assume that the gap is staggered as

\[
\frac{U}{2} \left( \langle n^T_{i\uparrow} \rangle - \langle n^T_{i\downarrow} \rangle \right) \equiv \begin{cases} +\Delta_{120} & \text{if } \lambda = \text{A, C, E} \\ -\Delta_{120} & \text{if } \lambda = \text{B, D, F} \end{cases}, \tag{14} \]

to form a 120°-AF order. Using the operators for sublattices, the Hartree-Fock Hamiltonian in the wave-number representation is given as,

\[
H_{HF} = \sum_{k,\sigma} \left( a^\dagger_{k,\sigma} a_{k,\sigma} - \frac{1}{2} \begin{pmatrix} A \end{pmatrix} \begin{pmatrix} a_{k,\sigma}^A \\ a_{k,\sigma}^B \\ a_{k,\sigma}^C \\ a_{k,\sigma}^D \\ a_{k,\sigma}^E \\ a_{k,\sigma}^F \end{pmatrix} - \frac{1}{2} \begin{pmatrix} \Omega \end{pmatrix} \right) \cdot \begin{pmatrix} \Omega^A \\ \Omega^B \\ \Omega^C \\ \Omega^D \\ \Omega^E \\ \Omega^F \end{pmatrix}, \tag{15} \]

FIG. 1: (Color online) Schematic representation of spin structure in two AF orders studied in this paper for the anisotropic triangular lattice: (a) an ordinary ($\pi, \pi$)-AF order, and (b) an AF order with 120° spin structure.

FIG. 2: (Color online) Schematic explanation of Hartree-Fock approximation for an AF order with 120° spin structure. In (a), it is shown how we divide the anisotropic triangular lattice into six sublattices (A-F) with different directions of a spin quantization axis, which are illustrated in (b): the axis of B (C,D,E,F,A) sublattice is obtained by turning that of A (B,C,D,E,F) sublattice by 60 degrees. For these sublattices, we suppose that the gap parameter is staggered, namely $\Delta_{120}$, $-\Delta_{120}$, $\Delta_{120}$, ... leading to the formation of a 120°-AF order in Fig. 1(b).
where $a^{\lambda \lambda}_{k, \sigma}$ is the Fourier transformation of $a^\dagger_{k, \sigma}$, and

$$
A_1 = -t \cos(\pi/6)(e^{-ikx} + e^{-iky}),
$$

$$
A_2 = -t' \cos(\pi/3)e^{-i(k_x+k_y)},
$$

$$
B_{1+} = t \sin(\pi/6)(e^{-ikx} + e^{-iky}),
$$

$$
B_{1-} = -t \sin(\pi/6)(e^{ikx} + e^{iky}),
$$

$$
B_{2+} = t' \sin(\pi/3)e^{-i(k_x+k_y)},
$$

$$
B_{2-} = -t' \sin(\pi/3)e^{i(k_x+k_y)}.
$$

(16)

As $\Psi_{120}$, we adopt the lowest-energy eigenvector obtained by diagonalizing eq. (15). However, we do not determine $\Delta_{120}$ by a self-consistent equation in the Hartree-Fock approximation, but optimize $\Delta_{120}$ as a variational parameter in $\Psi_{Q}^{120}$ simultaneously with the other parameters with respect to the original Hamiltonian eq. (11). If $\Delta_{120}$ is finite, all sublattices have staggered spin densities, constituting the 120° spin structure.

D. Variational Monte Carlo calculations

Generally, it is not easy to accurately calculate expectation values of a many-body wave function with analytic approaches. Here, we apply an optimization VMC method,[25] which effectively minimizes the variational energy and makes a virtually accurate evaluation, to the wave functions mentioned in this section. We have performed VMC calculations mainly for the lattice of $N = L \times L$ sites with $L = 10$ and 12. The conditions of calculations here are mostly the same as those in (I).

III. RESULTS

In [III A] we consider the energies of $\Psi_{Q}^{120}$ and $\Psi_{Q}^{120}$, and the critical behaviors appearing in them. In [III B] we show these critical behaviors indicate a metal-to-insulator transition. In [III C] we discuss the properties of the AF order in the insulating regime of $\Psi_{Q}^{120}$, and the eventual phase diagram. In [III D] we consider the BCS state with another pairing symmetries expected for the region of $t' \gtrsim t$.

A. Stability of coexisting state and 120°-AF state

We start with the energy reduction of the coexisting state $\Psi_{Q}^{120}$ and the 120°-AF state $\Psi_{Q}^{120}$ for $t' \sim t$. In Figs. 3(a)

and 3(b), the total energy per site $E$ is compared among $\Psi_{Q}^{120}$ ($E^{120}$), $\Psi_{Q}^{120}$ ($E^{120}$) and $\Psi_{Q}^{120}$ ($E^{d}$) for $t'/t = 0.8$ and $1.0$, respectively. For both values of $t'/t$, the curves of $E/t$ for the three states are almost indistinguishable from one another for small $U/t$, whereas they separate with cusps as $U/t$ becomes large. In fact, as we will see shortly, these cusps indicate metal-insulator transitions. For $t'/t = 0.8$, $E^{120}$ exhibits a cusp first at $U = U^{120}_{c} = 6.65 \pm 0.05t$ and becomes appreciably lower than both $E^{d}$ and $E^{120}$ for $U > U^{120}_{c}$. On the other hand, for $t'/t = 1.0$, $E^{120}$ exhibits a cusp first at $U = U_{c}^{120} = 7.65 \pm 0.05t$ and becomes the lowest for $U > U_{c}^{120}$. Thus, the lowest-energy state for large $U/t$ is switched from $\Psi_{Q}^{120}$ to $\Psi_{Q}^{120}$ in the range of $0.8 < t'/t < 1.0$. To see $t'/t$ dependence of $E/t$ in the insulating regime ($U > U_{c}$), we plot the total energies at $U/t = 12$ of various states in Fig. 4. For $t' < t'_{c} \sim 0.90t$, the coexisting state is the most stable,
the conductive regime, we introduce the condensation energy: $E_c = E^F - E$, where $E^F$ denotes the energy per site of the projected Fermi sea, $\Psi_Q = \mathcal{P}\Phi_F$, as the reference value. In Fig. 5 $E^{co}_c$, $E^{120}_c$ and $E^d_c$ are shown for three values of $t'/t$. Note that $E_c$ for every state is almost zero for $U < U_{c, min}^{\mu}$, where $U_{c, min}^{\mu}/t$ is shown by an arrow in each panel. This means that every state for $U < U_{c, min}^{\mu}$ almost reduces to a normal metallic state $\Psi_Q$. Here, it is important to recall that, as discussed in (1), [20] robust SC occurs only for $U_{\mu, onset}^{d} < U < U_{c}^{d}$, in which $E_c/t$ has a small but perceptible finite value. Although this tendency can be seen in $E^d_c/t$ for $t'/t = 0.6$ and $6 \lesssim U/t < 7.15$ [Fig. 5(a)], more stable $\Psi_Q^{co}$ covers the whole range of SC, namely, $U_{c, min}^{\mu} = U_{c}^{co} < U_{\mu, onset}^{d}$. Consequently, $\Psi_Q^d$ comes to have no chance to arise appreciable SC. We will return to this subject in III B.

B. Metal-insulator transitions

In this subsection, we study the critical behavior at $U = U_c$ found in $E^{co}$ and $E^{120}$ (cusps) in Fig. 3 and in $E_c^{co}$ and $E_c^{120}$ (sudden increases) in Fig. 5. Although we have not mentioned, in fact, $E_c^{co}$ and $E_c^{120}$ in Fig. 3 undergo clear hysteresis (dual-minimum behavior) near the cusps at $U_c$. This indicates a kind of first-order transition takes place at $U_c$. We will reveal the properties of this transition with various quantities.

First, we take up the doublon density,

$$D = \frac{1}{N_s} \sum_i \langle n_i \bar{n}_i \rangle = \frac{1}{N_s} \langle \mathcal{H}_{\text{int}} \rangle,$$

where $\mathcal{H}_{\text{int}}$ denotes the second (interaction) term of the
FIG. 6: (Color online) Density of doubly-occupied site (doublon) as a function of $U/t$ for the lowest-energy states: the coexisting state $\Psi_0^{co}$ for $t'/t = 0.4-0.8$, and the 120$^\circ$-AF state $\Psi_{Q}^{120}$ for $t'/t = 1.0$.  

In Fig. 6, we depict the charge structure factor, $N(q)$ for the same states with those in Fig. 7 is plotted along the same path: (a) Coexistence state $\Psi_0^{co}$ for $t'/t = 0.8$, and (b) 120$^\circ$-AF state $\Psi_{Q}^{120}$ for $t'/t = 1.0$. The open (solid) symbols denote the data for $U < U_c$ ($U > U_c$).  

In Fig. 7 the momentum distribution function, 

$$ n(k) = \frac{1}{2} \sum_{\sigma} \langle c_{k\sigma}^\dagger c_{k\sigma} \rangle, \quad (19) $$

of the lowest-energy states is plotted for $t'/t = 0.8$ ($\Psi_0^{co}$) and 1.0 ($\Psi_{Q}^{120}$). Discontinuities of $n(k)$ at $k_F$ in both sections, (0, 0)-(0, $\pi$) and (0, 0)-(0, $\pi$), are obvious for $U < U_c$ for both magnetic states, whereas $n(k)$ becomes smooth in both sections for $U > U_c$. Because the quasi-Fermi surface vanishes for $U > U_c$, we may consider that the states become non-metallic.

In Fig. 8 we depict the charge structure factor, 

$$ N(q) = \frac{1}{N_s} \sum_{i,j} e^{iq \cdot (R_i - R_j)} \langle N_i N_j \rangle - n^2, \quad (20) $$

with $N_i = n_{i\uparrow} + n_{i\downarrow}$, for the same states as those in Fig. 7. Similarly to the case of $\Psi_0^{co}$ studied in (1), $N(q)$ near the Fermi point $(0, 0)$ seems linear in $|q|$ for $U < U_c$, whereas the behaviors of $N(q)$ abruptly change to roughly quadratic in $|q|$ for $U > U_c$, regardless of $\Psi_0^{co}$ or $\Psi_{Q}^{120}$. It follows that the states are gapless in the charge sector and are conductive for $U < U_c$, but a charge gap opens for $U > U_c$ and they become insulating.

The above results of $D$, $n(k)$ and $N(q)$ indicate that in $\Psi_0^{co}$ and $\Psi_{Q}^{120}$, a first-order metal-to-insulator transition occurs at
Another noticeable difference is the behavior of the doublet-holon binding parameter $\mu$. The discontinuity of $\mu$ at $U_c$ is an order of magnitude smaller in $\Psi_Q^\text{AF}$ than in $\Psi_Q^0$, for $t'/t \leq 0.8$. This behavior is considered reasonable, again assuming the $(\pi, \pi)$-AF order in the insulating regime. As we studied before, the doublon-holon binding effect is intrinsic in the Néel background of $\Psi_{AF}$. Accordingly, $\mu$ in the correlation factor $P_Q$ plays a minor role for the $(\pi, \pi)$-AF state. This tendency becomes more thorough for $\Psi_Q^0 < \mu$ in $\Psi_Q^{120}$, inversely, drops to almost zero at $U_c$ and remains very small for $U > U_c$. Similarly, $\mu$ drops to almost zero at $U_c$ for $\Psi_Q^{120}$, and also for $\Psi_Q^0$. Thus, the doublon-holon binding factor is almost useless for $\Psi_Q^{120}$ in the insulating regime. However, in the insulating regime of $\Psi_Q^{120}$, doublons exist as shown in Fig. 8 and we have confirmed in the records of Monte Carlo sweeps that a doublon almost necessarily sits in a nearest-neighbor site of a holon. This indicates that the one-body HF state $\Psi_Q^{120}$ already has a sufficient doublon-holon binding effect for finite $\Delta_{120}$. At any rate, the binding (and unbinding) of a doublon to a holon must be the essence of Mott transitions.

To directly confirm the existence of long-range magnetic orders for $U > U_c$, we next discuss the behavior of the gap parameters, $\Delta_{AF}$ and $\Delta_{120}$, and the order parameter $m_s$. For $\Psi_Q^0$, the sublattice magnetization $m_s$ is given, as usual, by

$$m_s = \frac{1}{N_s} \left| \sum_j e^{iK R_j} \langle S_j^z \rangle \right|,$$

with $S_j^z = 1/2 \left( c_{j,\uparrow}^T c_{j,\downarrow} - c_{j,\downarrow}^T c_{j,\uparrow} \right)$. Similarly, we define $m_s$ for $\Psi_Q^{120}$ as,

$$m_s^{120} = \frac{1}{N_s} \left| \sum_j e^{iK R_j} \langle S_j^{\uparrow \downarrow} \rangle \right|,$$

with $S_j^{\uparrow \downarrow} = 1/2 \left( a_{j,\uparrow}^T a_{j,\downarrow} - a_{j,\downarrow}^T a_{j,\uparrow} \right)$. For $m_s^{120} > 0$, $\Psi_Q^{120}$ has a $120^\circ$-AF order. In Figs. 10(a) and (b), we show $\Delta_{AF}$ and $m_s$ of $\Psi_Q^{120}$ for three values of $t'/t$ ($\leq 0.8$). The behavior of these two quantities is similar; they are negligibly small for $U < U_c$, whereas they abruptly increase at $U = U_c$ and preserve the large magnitude for $U > U_c$. They are almost independent of the value of $t'/t$. We will turn to this point in the subsequent sections. Shown in Figs. 10(c) and (d) are $\Delta_{120}$ and $m_s^{120}$ of $\Psi_Q^{120}$ for $t'/t = 1.0$. Their $U/t$ dependence is basically the same as those of $\Psi_Q^0$, but the magnitude of $\Delta_{120}/t$ and $m_s^{120}$ is larger than that of $\Delta_{AF}/t$ and $m_s$. In this point, the $120$-degree AF order is not less steadfast than the $(\pi, \pi)$-AF order. The spin structure factor $S(q)$ is also checked (not shown), which has a sharp peak at $q = (2\pi/3, 2\pi/3)$ in the insulating regime of $\Psi_Q^{120}$, supporting the realization of the $120^\circ$ spin structure. Thus, we have confirmed that a firm magnetic long-range order always arises in the insulating regime at least for $t'/t < 1$.

Finally, we discuss the $d$-wave gap $\Delta_d$ and the $d$-wave SC
correlation function of the nearest-neighbor-site pairing:

\[ P_d(r) = \frac{1}{4N_{\text{site}}} \sum_{\tau, \tau'} \left( (-1)^{1-\delta(\tau, \tau')} \times \langle \Delta^\dagger_{\tau}(R) \Delta_{\tau'}(R + r) \rangle \right) , \tag{23} \]

where \( x \) and \( y \) denote the lattice vectors in the \( x \) and \( y \) directions, and \( \Delta^\dagger_{\tau}(R) \) is the creation operator of a nearest-neighbor singlet,

\[ \Delta^\dagger_{\tau}(R) = (c_{1}^{\dagger} c_{\tau+1}^{\dagger} + c_{\tau+1}^{\dagger} c_{\tau}^{\dagger})/\sqrt{2} . \tag{24} \]

Unless \( \Delta_d \) increases, \( P_d(r) \) does not increase, but the opposite does not hold, in contrast to the relation between \( \Delta_{AF} \) and \( m_s \). It is possible that finite \( \Delta_d \) indicates a non-SC singlet gap. \[ \text{In contrast, } P_d(r) \text{ is an good indicator of } d_{x^2-y^2}-\text{wave SC, and was studied in detail for } \Psi_Q^d \text{ in (I), which yielded a conclusion that SC arises for } t'/t \lesssim 0.7 \text{ within } \Psi_Q^d. \text{ Here, we consider the long-distance behavior of } P_d(r) \text{ by } P_d^{\text{ave}} \text{, which is the average of } P_d(r) \text{ only for } r = (x, L/2) \text{ and } (L/2, y) \text{ with } x, y = 0-L. \]

As shown in Fig. 11(a), \( \Delta_d \) for \( \Psi_Q^{co} \) is always substantially zero for \( U < U_c \). Accordingly, \( P_d(r) \) does not develop meaningfully the value of \( U = 0 \), even if \( U \) approaches \( U_c \), as shown in Figs. 11(b) and 11(c). This is in contrast with the case of \( \Psi_Q^d \). Thus, appreciable SC does not appear in the conducting regime. In the insulating regime, the \( d_{x^2-y^2} \)-wave singlet gap \( \Delta_d \) is still strongly suppressed in \( \Psi_Q^{co} \) [Fig. 11(a)], compared with in \( \Psi_Q^d \) [Fig. 4(c) in (I)], where \( \Delta_d/t \sim 1.2-1.3 \). It is found, like the case of \( \Psi_Q^d \), \( P_d(r) \) is very small and vanishes rapidly as \( L \) increases (not shown). Consequently, for \( U > U_c \), the \((\pi, \pi)\)-AF order is overwhelmingly dominant over the \(d_{x^2-y^2} \)-wave SC order; \( \Psi_Q^{co} \) in the insulating side can be regarded as an almost pure \((\pi, \pi)\)-AF insulating state. It means that \( \Psi_Q^{co} \) undergoes a simple first-order metal-to-(\(\pi, \pi\))-AF-insulator transition at \( U = U_c \) [29] for \( t'/t \leq 0.8 \).

In conclusion, there is no chance that robust \( d \)-wave SC or a nonmagnetic insulator appears within \( \Psi_Q^{co} \).

### C. Antiferromagnetic state and phase diagram

In this subsection, we consider the properties of the \((\pi, \pi)\)-AF state realized in the insulating regime of \( \Psi_Q^{co} \).

In (I), we found that the properties of \( \Psi_Q^d \) in the (nonmagnetic) insulating regime are almost independent of the frustration strength \( t'/t \) [cf. Fig. 4 for example]. This tendency becomes more strong in \( \Psi_Q^{co} \). As in Fig. 11(b), the renormalized frustration \( t'/t \) becomes nearly zero for \( U > U_c \), regardless of the model parameter \( t'/t \), namely, in the strong coupling regime, the effective band almost retrieves the nesting condition for the simple square lattice (\( t' = 0 \)), even for highly frustrated cases.

The other variational parameters in \( \Psi_Q^{co} \) are also almost independent of \( t'/t \), as seen in each panel of Figs. 9(a), 10(a) and 12(a), where all the data points for \( U > U_c \) are represented very well by a unique curve, regardless of \( t'/t \). Thus, the optimized \( \Psi_Q^{co} \) is not changed with the frustration strength, as long as \( U > U_c \).

In Fig. 4 the total energy for \( \Psi_Q^{co} \) in the insulating regime \((U/t = 12)\) is plotted as a function of \( t'/t \). Here, \( E^{\text{ins}} \) is almost constant, and the difference of \( E/t \) between \( t'/t = 0 \) and 1.2 is as small as 0.1%. This behavior is not trivial even if the wave function is not changed with \( t'/t \), because the \( t' \)-term in the Hamiltonian changes. To understand this result, we check the behavior of energy components; let \( E_t, E_d \) and \( E_{\text{AF}} \) be the contributions from the hopping in the \( t \)-bond and \( t' \)-bond directions, and from the onsite interaction \( U, \) respectively. We list the numerical data for \( t'/t = 0.8 \) in Table I as...
energy reduction due to the diagonal hopping or frustration, even if $t' = 0$ or $t'/t$ is substantially zero, indicating if we allow the band renormalization, the wave function is by far stabilized by retrieving the nesting condition for the simple square lattice at the cost of the energy reduction due to the diagonal hopping or frustration, even if $t'/t$ is considerably large.

It is natural to guess that this renormalization readily occurs in $\Psi^d_Q$, because the nesting condition is advantageous not only to the $(\pi, \pi)$-AF state but to the $d$-wave state, as discussed in (I). Anyway, in recalling the point (iv) itemized in [11] we notice that the band renormalization effect, namely the recovery of nesting, is essential to stabilize the $(\pi, \pi)$-AF state, as well as the $d$-wave singlet state. [23]

Finally, we discuss the ground-state phase diagram, which is reconstructed within $\Psi^d_Q$ and $\Psi^{20}_Q$ and depicted in Fig. 13. As compared with the diagram by $\Psi^d_Q$ and $\Psi^{20}_Q$ shown in Fig. 14 in (I), the area of the $(\pi, \pi)$-AF insulator extends to extremely large $t'/t (> 0.9)$ and to somewhat small $U/t$. In addition, the area of the $120^\circ$-AF insulator appears near the isotropic point $t'/t = 1$. We consider these tendencies are broadly consistent with the results for the $J-J'$ model ($U/t = \infty$), [10] in which the domain of $(\pi, \pi)$-AF continues to $t'/t > 0.8$. In Fig. 13 as $U/t$ increases, the boundary value in $t'/t$ between the $(\pi, \pi)$-AF and $120^\circ$-AF insulators tends to increase. This is probably because $\Psi^d_Q$ is stabilized by the $d$-wave gap $\Delta_d$, which rapidly increases for large $U/t$, as seen in Fig. 11(a). We consider that the above tendency of the boundary will be corrected by introducing an appropriate singlet gap also into $\Psi^{20}_Q$. As a result of the stabilization of magnetic phases, the domains of nonmagnetic insulating and of robust $d$-wave SC phases disappear, which occupy certain parts of the phase diagram made in (I) and also in recent studies of a variational cluster perturbation theory [6] and a

![FIG. 11](image1)

![FIG. 12](image2)

![FIG. 13](image3)
cellular dynamical mean field theory. [7]

D. Extention of pairing-gap form

From the argument in III C, we expect a state yielding a gain in $E_t$ overcomes $\Psi_{Q}^{c0}$ and $\Psi_{Q}^{d0}$ for large $t'/t$. In this subsection, we consider a couple of different pairing gaps, which seem suitable for $t' \gg t$, in the projected BCS function.

One has a specific gap parameter to the $t'$ direction ($\Delta_{d'}$), independent of $\Delta_s$ for the $t$ direction, \[ \Delta_k = \Delta_s(\cos k_x + \cos k_y) - \Delta_{d'} \cos(k_x + k_y), \] (25)

which we call “ext. s+d$_{xy}$ wave” ($\Psi_{Q}^{s+d} = \mathcal{P}\Psi_{s+d}$). This form of $\Delta_k$ has nodes near the $k_x$ and $k_y$ axes for $\Delta_s \sim \Delta_{d'}$ [see Fig. 14(b)], which resembles the nodes proposed by some experiments. \[ \Delta_k \] approaches the $d_{xy}$ wave of a one-dimensional character for $|\Delta_{d'}| \gg |\Delta_s|$. The other is a $d_{x^2-y^2}+i d_{xy}$ wave ($\Psi_{Q}^{d+id} = \mathcal{P}\Psi_{d+id}$),

\[ \Delta_k = \Delta_{d+id} \left[ \cos k_x + e^{i \frac{\pi}{4}} \cos(k_x + k_y) + e^{i \frac{\pi}{4}} \cos k_y \right], \] (26)

as shown in Fig. 14(c). This form was often used to study favorable gap symmetries for cobaltate SC; [32, 34] using a VMC method \[ \Psi_{Q}^{c0} \] for the $t$-$J$ model on an isotropic triangular lattice, it was shown that $\Psi_{Q}^{d+id}$ is degenerate with $\Psi_{Q}^{c0}$ at half filling, and has lower energy for doped cases. This gap form breaks a time reversal symmetry.

In Fig. 4, the total energies of $\Psi_{Q}^{s+d'}$ ($E_{s+d'}$) and $\Psi_{Q}^{d+id}$ ($E_{d+id}$) are plotted in addition to those mentioned earlier. For $t'/t \lesssim 1.1$, $E_{d+id}$ is almost constant in the same reason as $E_{c0}$ and $E_s$, whereas $E_{d+id}$ starts to decreases at $t'/t \sim \Delta_{d'}$ abruptly, because, there, the direction of band renormalization is reversed from $t'/t \rightarrow 0$ to $t'/t \rightarrow \infty$. Thus, the effective Fermi surface of $\Psi_{Q}^{d+id}$ becomes quasi one dimensional for $t'/t \gtrsim 1.1$. Similarly to $E_{d+id}$, $E_{s+d}$ considerably decreases as $t'/t$ increases. In the range of decreasing $E$, the energy reduction in both $\Psi_{Q}^{d+id}$ and $\Psi_{Q}^{s+d'}$ is largely attributed to $E_t$.

Especially in $\Psi_{Q}^{s+d'}$, the energy reduction is entirely owing to $E_t$, and the direction of band renormalization is $t'/t \rightarrow \infty$; the optimized $\Delta_s$ is negligible ($\sim 0.54$) compared to the optimized $\Delta_s'$ ($\sim 7.05$), for $U/t = 12$, $t'/t = 1.2$, and $L = 12$. Thus, the singlet gap has an almost pure $d_{xy}$-wave of one-dimensional character. As shown in Fig. 4, $E_{s+d}$ overcomes $E_{c0}$ for $t' \gtrsim t_{c2} \sim 1.65t$ for $U/t = 12$, meaning that $\Psi_{Q}^{d}$ is predominant for an unexpectedly large range of $t'/t (> 1)$ within the states we have studied ($L = 10$ and 12). We expect a more favorable pairing gap will be found for $t < t' < t_{c2}$, but we leave a search for it for the future.

Detailed results for $\Psi_{Q}^{s+d'}$ was reported in another publication. [40]

IV. CONCLUSION

A. Summary

As a continuation of the preceding study (I), [3] we have studied the Hubbard model on anisotropic triangular lattices, eq. (1), at half filling, using an optimization variational Monte Carlo method. We introduce two new trial wave functions:

1. A coexisting state of $(\pi, \pi)$-AF and $d$-wave gaps, which allows for a band renormalization effect, $\Psi_{Q}^{c0}$, and (ii) a state with an AF order of $120^\circ$ spin structure, $\Psi_{Q}^{d0}$. Main results are summarized as follows:

[1] First-order metal-to-insulator transitions occur in both $\Psi_{Q}^{c0}$ and $\Psi_{Q}^{d0}$ at smaller values of $U/t$ than those of the $d$-wave state $\Psi_{Q}^{d}$ studied in the preceding paper (I). As a result, the regime of robust $d$-wave SC found in (I) is covered with the domain of these states. The modified phase diagram within $\Psi_{Q}^{c0}$ and $\Psi_{Q}^{d0}$ is shown in Fig. 13.

[2] In the insulating regimes, $\Psi_{Q}^{c0}$ and $\Psi_{Q}^{d0}$ are considerably stable, compared with $\Psi_{Q}^{d}$, and magnetic long-range orders always exist for $t'/t \lesssim 1.65$. Thus, a domain of a non-magnetic insulator is not found for $t' \sim t$ within the wave functions used this time.

[3] In the insulating regime of $\Psi_{Q}^{c0}$, the realized state can be regarded as a pure $(\pi, \pi)$-AF insulator, because the sublattice magnetization as well as the $(\pi, \pi)$-AF gap ($\Delta_{AF}$) is robust, and the $d$-wave pairing correlation almost vanishes. In the optimized $\Psi_{Q}^{d0}$, the effective band is renormalized so greatly ($t' \rightarrow 0$), irrespective of $t'/t$, that the nesting condition for $t' = 0$ is retrieved almost completely. Accordingly, the contribution of diagonal hopping energy vanishes even for large $t'/t$.

[4] For $t' \sim t$, $\Psi_{Q}^{d0}$ becomes predominant ($U > U_c$), even though the effects of band renormalization and of coexisting singlet gaps are not considered. If these effects are introduced, the area of the $120^\circ$-AF order will somewhat expands, although, at present, the area of the $(\pi, \pi)$-AF order extends to as large as $t'/t \geq 0.9$.

[5] For large values of $t' (t > t_{c2} \sim 1.65)$, the singlet pairing states with gaps oriented to the diagonal-bond direction overcome $\Psi_{Q}^{d}$. We speculate that another predominant singlet (and SC) state will be discovered for $t < t' < t_{c2}$.

We believe that the mechanisms of a Mott (conductive-to-nonmagnetic insulator) transition and of the $d_{x^2-y^2}$-wave SC pursued in (I) fundamentally remain valid, if the magnetic orders are removed for some reasons. However, the ground-state
phase diagram for the model eq. 11 is substantially modified by $\Psi^0_Q$ and $\Psi^{120}_Q$.

B. Discussions

In comparing the present results with experimental ones of $\kappa$-ET salts, a favorable point is that a $\pi$, $\pi$-AF insulator is realized for realistic values of $t'/t$, namely e.g. 0.74 in $\kappa$-(ET)$_2$Cu[N(CN)$_2$]Cl. An unfavorable point is that robust SC and a nonmagnetic insulator do not appear; the latter state is considered to be realized in $\kappa$-(ET)$_2$Cu$_2$(CN)$_3$. One possible cause of this discrepancy is the insufficiency of trial wave functions; it is possible that quantum fluctuation is not a Gutzwiller approximation concluded that a $d+id$-wave SC is stable for $U \sim W$ and $t' \lesssim t$. Thus, it is urgent to carry out VMC calculations, in which the form of the pairing gap can be optimized without biased assumptions.

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Although robust SC does not appear within the present study, we found that the symmetry of a singlet gap changes at large $t'/t \sim 1.2$ from the simple $d_{x^2-y^2}$ wave to, for instance, the $d_{xy}$ wave as mentioned in (12) (see Fig. 4). This aspect is in accordance with that of FLEX, in which a predominant SC symmetry switches from a $d_{x^2-y^2}$ wave to a $d_{xy}$-wave state at $t'/t \sim 1$. Owing to this competition between $d_{x^2-y^2}$ and $d_{xy}$ waves near the isotropic point ($t'/t = 1$), the SC gap symmetry realized in $\kappa$-ET salts, especially in $\kappa$-(ET)$_2$Cu$_2$(CN)$_3$, may not be definitive but sensitive to physical parameters such as pressure. In contrast, a recent study of the Hubbard model with an extra exchange term using a Gutzwiller approximation concluded that a $d+id$-wave SC is stable for $U \sim W$ and $t' \lesssim t$. Thus, it is urgent to carry out VMC calculations, in which the form of the pairing gap can be optimized without biased assumptions.

Acknowledgments

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