Magnetic properties and Mott transition in the Hubbard model on the anisotropic triangular lattice

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Magnetic phase diagram and Mott transition are studied in the Hubbard model on the anisotropic triangular lattice at zero temperature and half-filling by the variational cluster approximation, taking into account Néel, 120° Néel, and collinear orderings. Paramagnetic insulator (spin liquid) is realized above the metallic phase around the isotropic point. In general, this spin liquid state, continuously connected with the metallic state, changes to a magnetic state as the on-site Coulomb repulsion \( U \) increases, but it persists up to large \( U \) limit in a small window between 120° Néel and collinear phases. For very large \( U \) another spin liquid state, separated from the metallic state by magnetic states, emerges around a narrow region where both Néel and 120° Néel orderings are highly suppressed due to the frustration and anisotropy. Implications for the \( \kappa \)-(BEDT-TTF)\(_2\)Cu\(_2\)(CN)$_3$ are discussed. As for the Mott transition, the structure of the self-energy in the spectral representation is studied in detail. As \( U \) increases around the Mott transition point, single dispersion evolves in the spectral weights of the self-energy which splits the non-interacting band into the upper and lower Hubbard bands.

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I. INTRODUCTION

When kinetic and Coulomb repulsion energies are competing, low dimensional materials with geometric frustration exhibit rich phenomena like superconductivity with various pairing symmetries, Mott transition, or pure paramagnetic insulator (spin liquid), which attract a lot of experimental and theoretical interests. The organic charge-transfer salts \( \kappa \)-(BEDT-TTF)$_2X$\(_3\)\(^{5-9}\) are good examples of such materials, where a transition from paramagnetic metal to spin liquid (Mott transition) has been detected with \( X=\text{Cu}_2(\text{CN})_3 \)\(^{10,11}\).

One of the important theoretical issues motivated by these experiments\(^{11-13}\) is the possibility of spin liquid phase compatible with experiments in the Hubbard model on the anisotropic triangular lattice described by the hopping \( t, t' \) and the on-site Coulomb repulsion \( U \) (see Fig. 1(a)), which is a simple effective Hamiltonian of these materials, and has been studied by various non-perturbative methods\(^{14,15}\).

Earlier studies\(^{5,9}\) reported that spin liquid is realized near the isotropic point \( t'/t = 1 \), however 120° Néel ordering (see Fig. 2 (b)), which is most relevant around \( t'/t = 1 \), was not considered in them. Taking into account 120° Néel ordering, the isotropic case \( t'/t = 1 \) is studied by the path integral renormalization group (PIRG)\(^{10}\) variational cluster approximation (VCA)\(^{11}\) and using effective models\(^{12,13}\) where PIRG study\(^{10}\) predicted that spin liquid is realized in the region \( 7.4 \lesssim U/t \lesssim 9.2 \), and the other studies\(^{11,12}\) also suggested the existence of spin liquid phase. For example, the VCA study\(^{11}\) argued that spin liquid is realized at least at \( U/t = 8 \). More generic ranges of \( t'/t \) are studied including 120° Néel ordering by the variational Monte Carlo (VMC)\(^{14,15}\) where the older study\(^{14}\) reported that spin liquid phase is not obtained for \( 0 \leq t'/t \leq 1.2 \) and \( 0 \leq U/t \leq 25 \), while the later study\(^{15}\) showed that spin liquid phase is not obtained at \( t'/t = 1 \), but it is realized around \( t'/t \approx 0.85 \) for \( 12 \lesssim U/t \). Therefore the conclusions about spin liquid in this model are very different not only depending on the approaches but also within the same approach.

In this paper, we investigate the magnetic properties and Mott transition in the Hubbard model on the anisotropic triangular lattice using VCA\(^{12,13}\) which is

\[ \begin{align*}
\text{FIG. 1: (Color online) (a) Anisotropic triangular lattice.} \\
\text{In our lattice geometry, the three sites 1, 2, and 3 form an} \\
\text{equilateral triangle of the unit length. The dotted hexagon is} \\
\text{the 12-site cluster used in our analysis. (b) The first Brillouin} \\
\text{zone of the anisotropic triangular lattice.}
\end{align*} \]
formulated based on a rigorous variational principle and exactly takes into account the short-range correlations. The three magnetic orderings, Néel, $120^\circ$ Néel, and collinear in Fig. 2, which are referred to as AF, spiral, and AFC hereafter, are considered and the 12-site cluster in the dotted hexagon in Fig. 1(a) is used. We study the phase diagram at zero temperature and half-filling, and show that for $0.8 \lesssim t'/t \lesssim 1.25$ paramagnetic metal changes to the spin liquid at $U/t = 6 \sim 7$, thus the (purely paramagnetic) Mott transition takes place there. This spin liquid state changes to a magnetic state at $U/t \lesssim 8$ for $0.8 \lesssim t'/t \lesssim 1.16$, but it persists up to large $U/t$ for $1.16 \leq t'/t \leq 1.23$ between spiral and AFC. For $15 \sim 20 \lesssim U$ there appears a narrow slit of spin liquid phase around $t'/t \approx 0.89$ where both AF and spiral orderings are highly suppressed due to the frustration and anisotropy. Implications of our analysis for experiments on the organic charge-transfer salts $\kappa$-(BEDT-TTF)$_2$X and analyses of the Heisenberg model are discussed. As for the Mott transition, the structure of the self-energy in the spectral representation is studied in detail. As $U$ increases around the Mott transition point, single dispersion evolves in the spectral weights of the self-energy which splits the non-interacting band into the upper and lower Hubbard bands.

II. HUBBARD MODEL ON THE ANISOTROPIC TRIANGULAR LATTICE

The Hamiltonian of the Hubbard model on the anisotropic triangular lattice reads

$$H = -\sum_{i,j,\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} - \mu \sum_i n_{i\sigma}, \quad (1)$$

where $t_{ij} = t$ for the solid lines and $t_{ij} = t'$ for the dashed lines in Fig. 1(a), $U$ is the on-site Coulomb repulsion, and $\mu$ is the chemical potential. The annihilation (creation) operator for an electron at site $i$ with spin $\sigma$ is denoted as $c_{i\sigma} (c_{i\sigma}^\dagger)$ and $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$. The energy unit is set as $t = 1$ hereafter.

We use VCA in our analysis. VCA is an extension of the cluster perturbation theory based on the self-energy-functional approach. This approach uses the rigorous variational principle $\delta \Omega_t[\Sigma] / \delta \Sigma = 0$ for the thermodynamic grand-potential $\Omega_t$ written as a functional of the self-energy $\Sigma$

$$\Omega_t[\Sigma] = F[\Sigma] + \text{Tr} \ln \left((G^{-1}_0 - \Sigma)^{-1}\right). \quad (2)$$

In the above expression, $F[\Sigma]$ is the Legendre transform of the Luttinger-Ward functional and the index $t$ denotes the explicit dependence of $\Omega_t$ on all the one-body operators in the Hamiltonian. The stationary condition for $\Omega_t[\Sigma]$ leads to the Dyson’s equation. All Hamiltonians with the same interaction part share the same functional form of $F[\Sigma]$, and using that property $F[\Sigma]$ can be evaluated from the exact solution of a simpler Hamiltonian $H'$, though the space of the self-energies where $F[\Sigma]$ is evaluated is now restricted to that of $H'$. In VCA, one uses for $H'$ a Hamiltonian formed of clusters that are disconnected by removing hopping terms between identical clusters that tile the infinite lattice. A possible symmetry breaking is investigated by including in $H'$ the corresponding Weiss field that will be determined by minimizing the grand-potential $\Omega_t$. Rewriting $F[\Sigma]$ in Eq. 2 in terms of the grand-potential $\Omega' = \Omega_t[\Sigma]$ and Green function $G''^{-1} = G_0^{-1} - \Sigma$ of the cluster Hamiltonian $H'$, the grand-potential is expressed as

$$\Omega_t(t') = \Omega' - \int d\omega C \sum_{\mathbf{k}} \ln \det \left(1 + (G_0^{-1} - G_0^{-1})G'\right)$$

and is now a function of $t'$, which denotes all the one-body operators in $H'$. The functional trace has become an integral over the diagonal variables (frequency and super-lattice wave vectors) of the logarithm of a determinant over intra-cluster indices. The frequency integral is carried along the imaginary axis and $\delta \to +0$. The stationary solution of $\Omega_t(t')$ and the exact self-energy of $H'$ at the stationary point, denoted as $\Sigma'$, are the approximate grand-potential and self-energy of $H$ in VCA, and physical quantities, such as expectation values of the one-body operators, are calculated using the Green function $G^{-1}_0 - \Sigma'$. In VCA, the restriction of the space of the self-energies $\Sigma$ into that of $H'$ is the only approximation involved and short-range correlations within the cluster are exactly taken into account by exactly solving $H'$.

In our analysis, the 12-site cluster in the dotted hexagon in Fig. 1(a) is used to set up the cluster Hamiltonian $H'$. On this cluster, the three sub-sites 1, 2, and 3 are treated on the same footing, and in the analyses of AF and AFC a ground state with equal number of up and down spins is possible. To study the magnetic orderings AF, spiral, and AFC, the Weiss field

$$H_{AF} = h_M \sum_i e_{a_i} \cdot \mathbf{S}_i \quad (3)$$

with the spin operator $\mathbf{S}_i = \sigma_{i\alpha} \sigma_{\alpha\beta} c_{i\beta}$ is included, where the index $a$ specifies the site in the unit cell in the sub-lattice formalism, and $a = 1, 2, 3$ for spiral, and $a = 1, 2$ for AF and AFC. For spiral order the unit vectors $e_{1,2,3}$ are oriented at $120^\circ$ each other, and for AF and AFC $e_1 = -e_2$ according to these spin orderings (see Fig. 2). In the stationary point search of $\Omega[(\mu', h_M)]$, which we denote as the grand-potential per site, the Weiss field $h_M$ and the cluster chemical potential $\mu'$ are treated as the variational parameters, where the latter should be included for the thermodynamic consistency. During the search, the chemical potential of the system $\mu$ is also adjusted so that the electron density $n$ is equal to 1 within 0.1%. In general, a stationary solution with $h_M \neq 0$ corresponding to the magnetically ordered state and that with $h_M = 0$ corresponding to the paramagnetic state (PM) are obtained, and the energies per site $E = \Omega + \mu n$
are compared for AF, spiral, AFC, and PM to determine the ground state. The density of state per site

\[ D(\omega) = \lim_{\eta \to 0} \int \frac{d^2k}{(2\pi)^2} \frac{1}{n_c} \sum_{\sigma,a=1}^{n_c} \left\{-\frac{1}{\pi} \text{Im} G_{\sigma\sigma}(k, \omega + i\eta)\right\} \]

is also calculated to examine the gap, where \( n_c \) is the number of the sites in the unit cell in the sense of the sub-lattice formalism (\( n_c = 3 \) for spiral, \( n_c = 2 \) for AF and AFC, and \( n_c = 1 \) for PM), and the \( k \) integration is over the corresponding Brillouin zone. In Eq. (4), \( \eta \to 0 \) limit is evaluated using the standard extrapolation method by calculating \( D(\omega) \) for \( \eta = 0.1, 0.05, \) and 0.025. The numerical error after this extrapolation is estimated to be of order \( 10^{-3} \), so the gap is identified as the region of \( \omega \) around \( \omega \approx 0 \) where the extrapolated \( D(\omega) \) is less than \( 10^{-2} \). We also compute the magnetic order parameter per site

\[ M = \frac{1}{n_c} \sum_{a=1}^{n_c} e_a \cdot \langle S_a \rangle \]

and the double occupancy per site

\[ D_{\text{occ}} = \frac{1}{n_c} \sum_{a=1}^{n_c} \langle n_{a\uparrow} n_{a\downarrow} \rangle = \frac{dE}{dU} \]

where \( \langle S_a \rangle \) and \( \langle n_{a\uparrow} n_{a\downarrow} \rangle \) are the expectation values of \( S_a \) and \( n_{a\uparrow} n_{a\downarrow} \), respectively.

FIG. 3: (Color online) Phase diagram of the Hubbard model on the anisotropic triangular lattice at zero temperature and half-filling as a function of \( t' \) and \( U \) obtained by VCA on the 12-site cluster. Lines are guides to the eye. The filled circles, triangles, and squares correspond to the AF, spiral and AFC transition points and crosses are the Mott transition points obtained assuming that no magnetic order is allowed. The line between AF and spiral phases is actually not a phase boundary, but spiral will change to AF through complicated (probably incommensurate) orderings. Energetically disfavored magnetic solutions, obtained only between the unfilled and filled circles, may be ground states with these complicated magnetic orderings.

FIG. 4: (Color online) The magnetic order parameter \( M \) for AF (filled-circles), spiral (filled-triangles) and AFC (filled-squares) at \( U = 30 \) as functions of \( t' \). The order parameters at \( U = 15 \) are also plotted as the unfilled marks for comparison.

III. PHASE DIAGRAM

Fig. 3 shows the phase diagram at zero temperature and half-filling obtained by VCA on the 12-site cluster, where the filled circles, triangles, and squares correspond to the AF, spiral and AFC transition points and crosses are the Mott transition points obtained assuming that no magnetic order is allowed (i.e. \( h_M = 0 \)). Energetically disfavored AF solutions are obtained between the unfilled and filled circles, and except this region, energetically disfavored magnetic solutions are not obtained.

Spin liquid (paramagnetic insulator) is realized above the Mott transition line for \( 0.8 \lesssim t' \lesssim 1.25 \), and it changes into magnetic states as \( U \) increases except in the range \( 1.17 \lesssim t' \lesssim 1.23 \), where this spin liquid phase persists up to large \( U \) limit.

In Fig. 3 the line between AF and spiral phases is actually not a phase boundary, and spiral order will gradually change to AF via complicated (probably incommensurate) magnetic orderings as \( t' \) decreases from the isotropic point \( t' = 1 \). These more complicated states will give local minimum (i.e. stationary solutions) with our choice of the Weiss fields since they will have orderings with AF or spiral like features, but their actual energies might be lower than the values computed with our Weiss fields. So these states may appear, not only as ground states, but also as energetically disfavored solutions, which may turn out to be ground states by more appropriate choice of Weiss fields. However, these energetically disfavored solutions are obtained only in the region between the filled and unfilled circles in Fig. 3 and most of the spin liquid phase in that phase diagram remains stable even if these energetically disfavored solutions are stabilized as discussed above.

In Fig. 3 the transition from the paramagnetic to magnetic states is of the second order except for \( 0.6 < t' < 0.9 \), since there exists no energetically disfavored magnetic solution outside the magnetic phase except this
range of \( t' \). If the energetically disfavored solutions in this range are stabilized as is discussed above, the magnetic transition is of the second order for all \( t' \). The Mott transition is of the second order since there is no energetically disfavored paramagnetic solution near the transition line. The Mott gap closes continuously at the transition point and the double occupancy is smooth there, as is shown later.

We have investigated the magnetic properties up to \( U = 30 \). Fig. 4 shows the AF (filled-circles), spiral (filled-triangles) and AFC (filled-squares) order parameter \( M \) at \( U = 30 \) as a function of \( t' \). The order parameter at \( U = 15 \) is also plotted as the unfilled marks for comparison. The spin liquid phase in Fig. 3 persists up to large \( U \) for \( 1.15 < t' < 1.24 \) (between the full and dash-dotted lines). The magnetic phase (AF and spiral) covers whole the region \( t' \leq 1.15 \) up to \( U \lesssim 15 \sim 20 \). For \( 20 \lesssim U \) there appears a very narrow slit of spin liquid phase around \( t' = 0.89 \) (between the dotted and full lines) where no magnetic solution (including energetically disfavored one) is obtained. This spin liquid state is separated from the metallic state by the magnetic states.

Here we consider the effects of the cluster size dependence quantitatively by comparing our results with the previous VAC study.\(^{11}\) performed at \( t'/t = 1 \). In general, as the cluster size increases, particles can move around wider space, which lowers the average kinetic energies and stabilizes metal, thus the critical interaction strength of the metal-insulator transition \( U_{MI} \) increases. Also, as the cluster size increases, spatial fluctuations are taken into account more and more, which destroy ordered phases, so the critical interactions strength of the magnetic transition \( U_c \) increases. This general argument suggests that both the magnetic and Mott transition lines in Fig. 3 will shift upwards in the thermodynamic limit. As for the Mott transition, \( U_{MI} \simeq 6.7 \) at the thermodynamic limit in Ref. \(^{11}\) which is in fact slightly larger than our 12-site value \( U_{MI} \simeq 6.3 \) in accordance with the above general argument, and gives us an estimate of the upper limit of the upward shift of our Mott transition line in Fig. 3. As for spiral order, it is argued in Ref. \(^{11}\) that spiral order is absent in the thermodynamic limit at least at \( U = 8 \), which is only very slightly smaller than our critical interaction strength \( U_c \simeq 8.1 \). This implies that our magnetic transition line in Fig. 3 can not shift downwards, again in accordance with the general arguments of the cluster size dependence. (The comparison of our order parameter with that of the Heisenberg analyses\(^{23-24}\) suggests that our magnetic transition line very likely shifts upwards. See below.) Therefore in the thermodynamic limit, the Mott transition line does not shift upwards by more than about 0.4, and the magnetic transition line does not shift downwards, but very likely shifts upwards in Fig. 3 and the main features of the phase diagram remain almost the same except the small upwards shift, in particular spin liquid is realized above the paramagnetic metal for \( 0.8 \lesssim t'/t \lesssim 1.25 \). The arguments and comparisons made above show that our results are quantitatively consistent with the previous VCA study.\(^{11}\)

Next we compare our results in the large \( U \) limit with the analyses\(^{23-24}\) of the Heisenberg model on the triangular lattice. Our value of the order parameter \( M = 0.528 \) at \( t'/t = 1 \) lies in the range \( 0.464 \leq M \leq 0.596 \) reported in Ref. \(^{23}\) (computed from \( M_c \)), and is larger than \( M \simeq 0.38 \sim 0.40 \) in Refs. \(^{24}\) which suggests that our 12-site VCA analysis still exaggerates the tendency of system to order and our magnetic transition line in Fig. 3 shifts upwards in the thermodynamic limit. A narrow spin liquid phase is predicted in the region \( 0.9 \lesssim t'/t \lesssim 0.95 \) (after translated in the large \( U \) limit) between AF and spiral in Ref. \(^{25}\). Spin liquid state is predicted around \( t'/t \sim 1.2 \) in Refs. \(^{25-26}\), though the ranges of \( t'/t \) vary depending on the analyses.\(^{23-26}\) Our results at \( U = 30 \) in Fig. 3 are consistent with these analyses.\(^{23-26}\) Contrary to these results, our spin liquid is not realized for \( t'/t \leq 1 \) in Refs. \(^{27}\). So conclusions on spin liquid state in the Heisenberg model seem to be still controversial. Since our VCA analysis still exaggerates the tendency of system to order and predicts disordered state (spin liquid), we speculate that our spin liquid phases in Fig. 3 remain even in the thermodynamic limit.\(^{23-26}\)

Next we compare our results with those in Refs. \(^{10-14,15}\). In the PIRG study\(^{10}\) performed at \( t'/t = 1 \), \( U_{MI} \sim 7.4 \) and \( U_c \sim 9.2 \), which are slightly larger than our values. In the VMC analysis of Ref. \(^{14}\) the region \( 0 \leq t' \leq 1.2 \) and \( 0 \leq U \leq 25 \) is studied but spin liquid phase is not obtained. The other VMC study\(^{15}\) reported that spin liquid phase is not realized at the isotropic point \( t' = 1 \), but it emerges around \( t' \approx 0.85 \) for \( 12 \leq U \) above the magnetic phase as \( U \) increases, and covers the region \( 0.7 \lesssim t' \lesssim 0.98 \) at \( U \sim 30 \). In the VMC analyses\(^{14,15}\) \( U_{MI} \) is larger than ours (e.g., \( 8 \lesssim U_{MI} \) at \( t' = 1 \) in them), and most of our spin liquid phase in Fig. 3 is metal in their phase diagrams. Our results in Fig. 4 are quali-

![FIG. 5: (Color online) The Mott gap \( \Delta \) (triangles) and double occupancy \( D_{occ} \) (circles) as functions of \( U \) at \( t' = 0.85 \).](image-url)
IV. MOTT TRANSITION

Next we study the Mott transition in detail. Fig. 5 shows the Mott gap $\Delta$ and double occupancy $D_{\text{occ}}$ as functions of $U$ at $t'/t = 0.85$ obtained assuming that no magnetic order is allowed (i.e. $h_M = 0$). The Mott gap closes continuously at the transition point and the double occupancy is smooth there.

In general, Mott transitions are predicted to be of the second order in VCA\textsuperscript{21}\textsuperscript{22} while they are predicted to be of the first order in the variational cluster approach with both degrees of freedom, where hybridization between the bath sites and cluster sites is treated as a variational parameter\textsuperscript{23}\textsuperscript{24} and the coexisting metal and insulator solutions, leading to the first order transition, differ by the value of this hybridization parameter. VCA analyses do not have both degrees of freedom and this technical difference may be the origin of the discrepancy.

Fig. 6 shows the momentum distribution function $n_k$ at $t' = 0.85$ along the dotted line in Fig. 1(b) for $U = 0$ (crosses), $U = 4$ (circles), and $U = 8$ (triangles). tentatively consistent with the recent VMC study\textsuperscript{25} in the sense that spin liquid emerges above the magnetic states as $U$ increases. But this spin liquid phase in the VMC\textsuperscript{26} is significantly wider than ours.

As for the disordered state of $\kappa$-(BEDT-TTF)$_2$Cu$_2$(CN)$_3$, an accurate estimation of $t'/t$ and $U/t$ seems to be very difficult. For example, $t'/t \simeq 1.1$ in Ref. 28 while $t'/t \simeq 0.83$ in Refs. 29\textsuperscript{30} and $5 \lesssim U/t \lesssim 8$ in Refs. 28\textsuperscript{29} while $12 \lesssim U/t \lesssim 15$ in Ref. 30. Unless $t'/t \lesssim 1$ and $U/t \simeq 15$, the spin liquid state of this material corresponds to the spin liquid in Fig. 3 which is realized $0.8 \lesssim t' \lesssim 1.25$ and continuously connected with the metallic state. If $t'/t \lesssim 1$ and $U/t \simeq 15$, the spin liquid state of this material corresponds to the spin liquid of the left side in Fig. 4 which is separated from the metallic state by the magnetic state. These qualitatively different two situations can be distinguished in experiments to see if the spin liquid state changes to the metal by, for example, continuously deforming the material and moving the system downwards in the phase diagram.

Next we study in detail the spectral density of the self-energy. The usual spectral density is defined by the Green function $G(k\sigma, z)$ as

$$A(k\sigma, \omega) = -\frac{1}{\pi} \text{Im} G(k\sigma, \omega + i\eta), \quad \text{(5)}$$

where $G(k\sigma, z)$ is expressed as

$$G(k\sigma, z) = \frac{1}{z - (\varepsilon_k - \mu) - \Sigma(k\sigma, z)} \quad \text{(6)}$$
in terms of the free band $\varepsilon_k$, $\mu$, and the self-energy $\Sigma(k\sigma, z)$. The self-energy is expressed in the spectral representation\textsuperscript{19} as

$$\Sigma(k\sigma, z) = g_{k\sigma} + \int_{-\infty}^{\infty} \frac{\sigma_{k\sigma}(\xi)}{z - \xi} d\xi, \quad \sigma_{k\sigma}(\xi) \geq 0. \quad \text{(7)}$$

and its spectral density is defined by

$$A_{\Sigma}(k\sigma, \omega) = -\frac{1}{\pi} \text{Im} \Sigma(k\sigma, \omega + i\eta). \quad \text{(8)}$$

For the Hamiltonian

$$g_{k\sigma} = U \langle n_{-\sigma} \rangle, \quad \int_{-\infty}^{\infty} \sigma_{k\sigma}(\xi) d\xi = U \langle n_{-\sigma} \rangle (1 - \langle n_{-\sigma} \rangle),$$

where $\langle n_{\sigma} \rangle$ is the average number per site of particles with spin $\sigma$ in the ground state.\textsuperscript{26} Here we consider the paramagnetic state at half-filling $\langle n_{\pm\sigma} \rangle = 1/2$ for large $U$ and set $\mu = U/2$, which cancels $g_{k\sigma} = U/2$ of Eq. (7) in Eq. (9).

When the spectral weight $\sigma_{k\sigma}(\xi)$ is dominated by single pole of the dispersion $\xi_k$, the Green function is given by

$$G(k\sigma, z) = \frac{1}{z - \varepsilon_k - \frac{U^2/4}{z - \xi_k}}, \quad \text{(9)}$$

whose poles are $\omega_{\pm} = (\varepsilon_k + \xi_k \pm U)/2$ for $U \gg |\xi_k|, |\xi_k|$, and the original band $\varepsilon_k$ splits into the upper and lower Hubbard bands (of almost equal weights) with a width of $U$. (The atomic limit $t' = 0$ yields the self-energy of the form in Eq. (9) with $\xi_k = 0$, which suggests that $\xi_k$ will be almost independent of $U$ for large $U$.)

Fig. 7 shows the spectral functions $A(k, \omega)$ and $A_{\Sigma}(k, \omega)$ calculated with $\eta = 0.1$ at $t' = 0.85$ for (a) $U = 6$, (b) $U = 8$, (c) (d) $U = 6.5$, and (e) (f) $U = 5$, assuming that no magnetic order is allowed. The non-interacting band is plotted with the full lines. At $U = 5$, which is slightly below the Mott transition point, small weights appear in $A_{\Sigma}(k, \omega)$ in (f) whenever the non-interacting band (full line) crosses the Fermi energy. At $U = 6.5$, which is slightly above the Mott transition point, these weights grows and begins to form single dispersion in (d).
FIG. 7: (Color online) The spectral functions $A(k, \omega)$ and $A_\Sigma(k, \omega)$ calculated with $\eta = 0.1$ at $t' = 0.85$ for (a) (b) $U = 8$, (c) (d) $U = 6.5$, and (e) (f) $U = 5$, assuming that no magnetic order is allowed. The full lines are the non-interacting ($U = 0$) band structure.

Corresponding to this growth of the weights at the Fermi surface in $A_\Sigma(k, \omega)$, a small gap opens at the Fermi surface in $A(k, \omega)$ in (c). In fact, as was calculated in Fig. 5 a small insulating gap opens simultaneously all over the whole Fermi surface at $U = 6.5$. As $U$ increases further, this dispersion in $A_\Sigma(k, \omega)$ dominates more and more in (b), splitting the upper and lower Hubbard band in (a).

V. SUMMARY AND CONCLUSIONS

In summary we have investigated the phase diagram of the Hubbard model on the anisotropic triangular lattice at zero temperature and half-filling by VCA. Spin liquid (paramagnetic Mott insulator) is realized for $0.8 \lesssim t'/t \lesssim 1.25$ above the metal-insulator (Mott) transition, which takes place around $U/t \approx 6$. This spin liquid phase, continuously connected with the metal, changes into the magnetic phase around $U/t \approx 8$ for $0.8 \lesssim t'/t \lesssim 1.16$, while it persists up to large $U/t$ for $1.16 \lesssim t'/t \lesssim 1.23$, separating spiral and AFC phases. For $15 \sim 20 \lesssim U$ there appears a narrow slit of spin liquid phase around $t'/t \approx 0.89$ where both AF and spiral orders are highly suppressed due to the anisotropy. This spin liquid phase is separated from the metal by the magnetic states.

The spin liquid state of the organic charge-transfer
salts $\kappa$-(BEDT-TTF)$_2$Cu$_2$(CN)$_3$ corresponds either of these qualitatively different spin liquid states, which can be experimentally distinguished by continuously deforming the material and moving the system downwards in the phase diagram.

The detailed comparisons of our results with those of the previous VCA\cite{11} and Heisenberg studies\cite{21} (both performed at $t'/t = 1$) indicate that the main features of our phase diagram Fig. 3 remain almost the same and the spin liquid phases in Fig. 4 are stable in the thermodynamic limit.

As for the Mott transition, the structure of the self-energy in the spectral representation is studied in detail. As $U$ increases around the Mott transition point, single dispersion evolves in the spectral weights of the self-energy, which splits the non-interacting band into the upper and lower Hubbard bands near the Fermi level.

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