Thermal algebraic-decay charge liquid driven by competing short-range Coulomb repulsion

Ryui Kaneko,1,2,∗ Yoshihiko Nonomura,2 and Masanori Kohno2,3

1 Institute for Solid State Physics, University of Tokyo, Kashiwa 277-8581, Japan
2 International Center for Materials Nanoarchitectonics (WPI-MANA), National Institute for Materials Science, Tsukuba 305-0044, Japan
3 Research Center for Functional Materials, National Institute for Materials Science, Tsukuba 305-0003, Japan

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We explore the possibility of a Berezinskii-Kosterlitz-Thouless-like critical phase for the charge degrees of freedom in the intermediate-temperature regime between the charge-ordered and disordered phases in two-dimensional systems with competing short-range Coulomb repulsion. As the simplest example, we investigate the extended Hubbard model with on-site and nearest-neighbor Coulomb interactions on a triangular lattice at half filling in the atomic limit by using a classical Monte Carlo method, and find a critical phase, characterized by algebraic decay of the charge correlation function, belonging to the universality class of the two-dimensional XY model with a $Z_6$ anisotropy. Based on the results, we discuss possible conditions for the critical phase in materials.

I. INTRODUCTION

Topological states have recently attracted increasing attention in search of novel states of matter in materials. Topological insulators [1], topological superconductors [2], quantum Hall systems [3], Kitaev-model systems [4], symmetry-protected topological states [5, 6], and Haldane-gap systems [7, 8] exhibit features characterized by topology. The Berezinskii-Kosterlitz-Thouless (BKT) phase is also a topological phase which exhibits power-law decay of the correlation function in contrast to a high-temperature disordered phase exhibiting an exponential decay or a low-temperature long-range ordered phase [9, 10]. Although the BKT phase is known to appear in the Coulomb gas model with long-range (logarithmic) interactions or in planar classical spin systems in two spatial dimensions, our motivation is to explore a BKT-like critical insulating phase for the charge degrees of freedom with short-range Coulomb repulsion. We consider the following conditions for the critical phase: (i) two spatial dimensions in favor of topological features, (ii) competing Coulomb interactions that cause degeneracy for charge configurations, and (iii) intermediate temperature which is not too low to stabilize charge order and not too high to result in a disordered state. As the simplest model, we consider the extended Hubbard model with on-site and nearest-neighbor Coulomb interactions on a triangular lattice. This model has been investigated using numerical simulations primarily at zero temperature and properties of it have been discussed particularly in relation to organic materials [11–22] and adatoms on semiconductor surfaces [23–27]. On the other hand, nonzero-temperature properties of the model have drawn little attention so far. Possible critical behavior as well as the finite-temperature phase diagram has never been investigated before. In the present paper we focus attention on the half filling in the insulating atomic limit by neglecting the hopping term. This simplification removes complexity arising from the fermionic degrees of freedom and allows us to apply a numerically exact classical Monte Carlo method to large systems at nonzero temperatures, and to uncover the presence of the charge BKT-like critical phase in the strongly correlated region of the two-dimensional Hubbard model, as shown in Fig. 1.

The present paper is organized as follows: In Sec. II, we introduce the extended Hubbard model in the atomic limit on a triangular lattice. In Sec. III, we present details of the finite-temperature phase diagram (Fig. 1), and show charge properties in each phase. We offer the numerical evidence of the BKT-like critical phase for the charge degrees of freedom and discuss its nature. Moreover, we explain how the spin degrees of freedom modify the phase diagram in the extended Hubbard model by

![Phase diagram](image_url)

FIG. 1. Phase diagram of the extended Hubbard model with on-site and nearest-neighbor Coulomb interactions in the atomic limit obtained by Monte Carlo calculations. The parameters $U(> 0)$ and $V(> 0)$ denote the on-site and nearest-neighbor Coulomb repulsion, respectively, and $T$ indicates temperature. The first-order transition line (double line) separates the charge-ordered and disordered phases, and bifurcates at the critical end point (open circle) into the boundaries (single lines) of the critical phase.
II. MODEL AND METHOD

A. Extended Hubbard model

We consider the extended Hubbard model on a triangular lattice in the atomic limit. The Hamiltonian reads

\[ H_{EH} = U \sum_i n_{i\uparrow} n_{i\downarrow} + V \sum_{\langle i,j \rangle} n_{i\sigma} n_{j\sigma} - \mu \sum_i n_i, \]

where \( U \) (\( V \)) denotes the strength of on-site (nearest-neighbor) Coulomb interaction, and \( \mu \) indicates chemical potential. Here \( n_i = n_{i\uparrow} + n_{i\downarrow} \), and \( n_{i\sigma} \in \{0, 1\} \) denotes the number of electrons with spins \( \sigma = \uparrow, \downarrow \) at site \( i \), and \( \langle i,j \rangle \) means that sites \( i \) and \( j \) are nearest neighbors. The electron density is given by

\[ \rho = \frac{1}{N_e} \sum_i \langle n_i \rangle, \]

where \( N_e \) and \( \langle \cdots \rangle \) denote the system size and thermal averaging, respectively. We consider the half-filled case \( \rho = 1, \mu = U/2 + zV \) with the coordination number \( z = 6 \) on a triangular lattice). Hereafter, we focus on the repulsive Coulomb interactions \((U, V > 0)\).

B. Classical Monte Carlo method

We apply the classical Monte Carlo method with the local-update Metropolis algorithm to investigate the phase diagrams for the extended Hubbard model. A similar approach has been applied to the doped systems on a triangular lattice [32, 33]. We perform the grand-canonical Monte Carlo simulation containing insertion and removal of electrons as well as moving of them [29]. We also use the exchange Monte Carlo method [34] to perform the simulation at low temperatures efficiently. We typically use 200 or 400 replicas distributed evenly in the temperature region \( 0 < T/V \leq 1 \). We adopt the periodic boundary condition, and consider the system size \( N_e = L^2 \) with \( L = 12, 24, 48, 96, \) and \( 192 \). We typically perform \( 10^5 \) Monte Carlo steps for sampling after discarding \( 10^4 \) Monte Carlo steps for thermalization. We perform 10 independent runs starting from different random initial conditions to estimate statistical errors. Hereafter, we will set the Boltzmann factor \( k_B = 1 \), and choose \( V \) as the unit of energy in the extended Hubbard model.

III. RESULTS

A. Ground states

Before discussing the phases at nonzero temperatures of the extended Hubbard model, let us discuss the ground states. When the on-site Coulomb interaction \( U \) is much larger than \( V \), the double occupancy of electrons is prohibited and the ground state is charge uniform, where all sites are singly occupied. On the other hand, when the nearest-neighbor Coulomb interaction \( V \) is much larger than \( U \), empty sites reduce the energy loss in the \( \sum_i n_i n_j \) term. As a result, the ground state becomes the \( 012 \)-type charge-ordered state where three-sublattice sites have \( n_i = 0, 1, \) and \( 2 \) (see the left side of Fig. 2). Note that the same charge order configuration is found in the presence of nonzero hopping [25, 26, 35]. The energy per site for the former state is \( E/N_e = 3V \) while that for the latter state is \( E/N_e = 2V + U/3 \), and hence, the level crossing occurs at \( U/V = 3 \) (see a schematic ground-state phase diagram in Fig. 2). Hereafter, we mainly focus on the realistic parameter region \( U \gtrsim V \).

Note that the classical ground state has macroscopic degeneracy exactly at \( U = 0 \). Each local triangle can have one of the \{012, 002, 022\} charge configurations with the conserved total number of electrons. Besides, in the presence of very strong attractive on-site Coulomb interaction \((U \to -\infty)\), electrons bind together, and singly occupied sites disappear. The achievable number of electrons per site is only \( n_i = 0 \) or \( 2 \), and the system effectively becomes the antiferromagnetic Ising model on a triangular lattice [36]. The correlation function of the Ising order parameter \((n_i - 1)\) in this case shows the power-law decay \( \sim 1/r^\eta \) as a function of distance \( r \) with the critical exponent \( \eta = 1/2 \) at zero temperature [37, 38].

B. Phase diagram at nonzero temperatures

Reflecting the charge order in the ground state, the ordered phase survives at nonzero temperatures for \( U/V <
The first-order phase transition occurs from the ordered phase to the disordered phase along the transition line for $U_c/V < U/V < 3$. The first-order transition line bifurcates at the critical end point $(U_c/V, T_c/V) = (2.45(5), 0.36(1))$ into two boundaries which enclose a critical phase. The boundaries are determined from the behavior of the charge correlation function which will be explained in Sec. III E.

To get insight into the charge critical phase, we show temperature dependence of the sublattice charge order parameter $N_{\text{sub}}$. Here the electron density for each sublattice $n_{\alpha}$ ($\alpha = A, B, C$) on a triangular lattice is defined by

$$n_{\alpha} = \frac{3}{N_s} \sum_{i \in \alpha} n_i.$$  

At low temperatures, the 012-type charge order develops, and $N_{\text{sub}}$ approaches $5 = 0^2 + 1^2 + 2^2$. At high temperatures, charge becomes uniform, each site contains one electron, and $N_{\text{sub}}$ approaches $3 = 1^2 + 1^2 + 1^2$. By contrast, in the intermediate (shaded) region between the charge-ordered and disordered phases in Fig. 3(a), $N_{\text{sub}}$ shows a large size dependence, and seems to approach 3 extremely slowly. This fact suggests the presence of an intermediate region, where the charge correlation shows nearly critical behavior.

Just above and below the intermediate phase, the specific heat defined by

$$C = \frac{\langle H_{\text{EH}}^2 \rangle - \langle H_{\text{EH}} \rangle^2}{T^2}$$  

shows broad two peaks, as shown in Fig. 3(b). Although the position of the lower-temperature peak at $T/V \approx 0.3$ is almost independent of sizes, that of the higher-temperature peak at $T/V \approx 0.6$ approaches lower temperatures as the system size increases. Nevertheless, the peak values do not change significantly, which suggests that this behavior is a crossover or a BKT-like transition.

C. Density of doubly occupied sites

We also calculate temperature dependence of the density of doubly occupied sites defined by

$$\rho_2 = \frac{1}{N_s} \sum_i \langle n_{i\uparrow} n_{i\downarrow} \rangle,$$  

as shown in Fig. 4. At half filling, the density of empty sites $\rho_0 = 1$ and doubly occupied sites are simultaneously created when an electron with a spin $\sigma$ moves from a singly occupied site to another singly occupied site. Thus, the density of singly occupied sites is given as $\rho_1 = 1 - 2\rho_2$. In the 012-type charge-ordered state at zero temperature, $\rho_0 = \rho_1 = \rho_2 = 1/3$. In the high-temperature limit, since all the interactions can be neglected, $\rho_0 = \rho_1 = \rho_2 = 1/4$, where the density of singly occupied sites by a spin $\sigma$ electron is denoted by $\rho_{2\sigma}$. Here $\rho_{1\uparrow} = \rho_{1\downarrow} = \rho_1/2$ without magnetic field. Remarkably, $\rho_2$ is not monotonic as a function of $T$, and becomes a maximum in the critical phase.

For further understanding of the behavior of charge, we show the snapshots of charge configuration in the real space in Fig. 5. As the temperature is raised, the 012-type charge order [see Fig. 5(a)] in the low-temperature regime is partially broken by thermal fluctuations, and 002 or 022 triangles [see Fig. 5(b)] are induced in the intermediate-temperature regime. Thus, $\rho_1$ decreases, while $\rho_2 = (1 - \rho_1)/2$ increases (see Fig. 4). On the other hand, in the high-temperature regime, the charge distribution becomes more random [see Fig. 5(c)], and $\rho_1$ ($\rho_2$) increases (decreases) (see Fig. 4).

While the charge particles themselves interact with each other with the logarithmic potential in the two-dimensional Coulomb gas model, defects surrounded by ordered domains correspond to the vortices and antivortices in the present critical phase, and the topological nature of it should be equivalent to that found in Ising antiferromagnets on a triangular lattice [39].
D. Emergent U(1) symmetry

To see the U(1) symmetry induced by thermal fluctuation in the critical phase, we define the radius variable $R$ and azimuth variable $\theta$ as

\begin{align}
N_x + iN_y &= R e^{i\theta}, \\
R &= \sqrt{N_x^2 + N_y^2}, \\
\text{and } \theta &= \arctan \frac{N_y}{N_x}
\end{align}

with

\begin{align}
N_x &= \frac{2n_A - n_B - n_C}{\sqrt{6}} \\
\text{and } N_y &= \frac{n_B - n_C}{\sqrt{2}}
\end{align}

by using the electron density for each sublattice $n_\alpha$ ($\alpha = A, B, C$) in Eq. (4). The equivalent variables for the spin degrees of freedom have been used in previous studies, especially, in Ising antiferromagnets on a triangular lattice [39–45].

The charge-ordered states are sixfold degenerate, and we can assign the radius and azimuth variables to each state, as shown in Table I and Fig. 6. The squared radius is proportional to the charge structure factor at the ordering wave vector $Q = (4\pi/3,0), (2\pi/3,2\pi/\sqrt{3})$ on the hexagonal Brillouin zone:

\begin{align}
\langle R^2 \rangle &= \frac{1}{3} ((n_A - n_B)^2 + (n_B - n_C)^2 + (n_C - n_A)^2) \\
&= 6N(Q) / N_s,
\end{align}

where the charge structure factor $N(Q)$ is defined by

\begin{equation}
N(Q) = \frac{1}{N_s} \sum_{i,j} (\langle n_i n_j \rangle - \rho^2) e^{iQ \cdot (r_i - r_j)}.
\end{equation}

When the long-range order appears, the azimuths satisfy $\langle \cos 6\theta \rangle = -1$, and the squared radius $\langle R^2 \rangle$ gives a nonzero value in the thermodynamic limit.

The ground state is characterized by the radius $R = \sqrt{2}$ and the azimuths $\theta = \pi/6 + n\pi/3$ ($n \in \mathbb{Z}$) (see Table I). As shown in Fig. 7, these azimuths appear more frequently at sufficiently low temperatures, and the six
TABLE I. Radius and azimuth variables for the sixfold-degenerate ground states (see Fig. 6) of the charge degrees of freedom.

| State # | 1    | 2    | 3    | 4    | 5    | 6    |
|---------|------|------|------|------|------|------|
| \(n_A\) | 2    | 1    | 0    | 0    | 1    | 2    |
| \(n_B\) | 1    | 2    | 2    | 1    | 0    | 0    |
| \(n_C\) | 0    | 0    | 1    | 2    | 2    | 1    |
| \(N_x\) | +3/\(\sqrt{6}\) | 0 | -3/\(\sqrt{6}\) | -3/\(\sqrt{6}\) | 0 | +3/\(\sqrt{6}\) |
| \(N_y\) | +1/\(\sqrt{2}\) | +\(\sqrt{2}\) | +1/\(\sqrt{2}\) | -1/\(\sqrt{2}\) | -\(\sqrt{2}\) | -1/\(\sqrt{2}\) |
| \(R\)   | \(\sqrt{2}\) | \(\sqrt{2}\) | \(\sqrt{2}\) | \(\sqrt{2}\) | \(\sqrt{2}\) | \(\sqrt{2}\) |
| \(\theta\) | +\(\pi/6\) | +\(\pi/2\) | +5\(\pi/6\) | -5\(\pi/6\) | -\(\pi/2\) | -\(\pi/6\) |

FIG. 6. Radius and azimuth variables for each charge-ordered state. The state number in each triangle corresponds to that in Table I. Large, middle, and small circles represent the sites with \(n_i = 2\), \(n_i = 1\), and \(n_i = 0\), respectively.

peaks develop in the histogram, corresponding to the charge order of the ground state. As temperature increases, the peaks broaden and become indiscernible.

The behavior of charge melting is visualized more clearly in the histogram of the two-component vector \((N_x, N_y)\). At a low temperature \((T/V = 0.325)\), the six sharp peaks appear at \(R \simeq \sqrt{2}\) and \(\theta = \pi/6 + n\pi/3\) \((n \in \mathbb{Z})\) [see Fig. 8(a)]. At an intermediate temperature \((T/V = 0.45)\), a ring structure develops instead of the discrete peaks. This behavior suggests the melting of charge order and the emergence of U(1) symmetry by thermal fluctuations [see Fig. 8(b)], and the radius \(R\) shrinks as temperature increases. At a high temperature \((T/V = 0.7)\), \(R\) becomes nearly zero, which suggests absence of the long-range order [see Fig. 8(c)]. Note that \(\langle R^2 \rangle\) is scaled with \(L^{-\eta}\) \((\eta > 0)\) for large \(L\) in the intermediate-temperature region (see Sec.III E).

Such an emergent U(1) symmetry has been discussed in the two-dimensional \(p\)-state clock model, which is a discrete version of the XY model [46]. For \(p \to \infty\), the system is identical to the XY model, and the BKT phase appears at nonzero temperatures. For a finite but large enough \(p\), thermal fluctuations effectively smear out discreteness of the order parameter, and still induce the BKT phase. At the same time, long-range order remains at finite temperatures. The renormalization-group analysis [46] suggests that two BKT transitions appear for \(p > p_c\) with 4 < \(p_c\) < 5. The present system would correspond to the case of \(p = 6\), which is above the critical value \(p_c\).

E. Critical exponent

Here we investigate the critical behavior of the BKT-like transitions to show that the intermediate phase can be identified with that of the two-dimensional XY model with a \(\mathbb{Z}_6\) anisotropy.

In the critical region, the charge correlation function shows algebraic decay as a function of distance \(r\) with the critical exponent \(\eta\):

\[
\langle n_0 n_r \rangle - \rho^2 \sim r^{-\eta}.
\]  

(14)

Then, the peak value of charge structure factor is scaled as

\[
N(Q) = \sum_r \langle n_0 n_r \rangle - \rho^2 e^{iQr} 
\sim \int_{-\Lambda}^{\Lambda} d^2r r^{-\eta} \sim L^{2-\eta},
\]  

(15)

where \(\Lambda\) is a cutoff, and the squared radius [Eq. (12)]
The critical exponent \( \eta \) shows the power-law decay as
\[
\langle R^2(L) \rangle \sim L^{-\eta}.
\] (16)
The critical exponent \( \eta \) can be estimated \([47]\) by \( \eta = \lim_{L_1, L_2 \to \infty} \eta(L_1, L_2) \) with
\[
\eta(L_1, L_2) = -\frac{\ln\langle R^2(L_2) \rangle / \langle R^2(L_1) \rangle}{\ln(L_2/L_1)}.
\] (17)

As shown in Fig. 9, \( \eta \) approaches zero at low temperatures because \( \langle R^2 \rangle \) converges to a nonzero value \([\text{see Eqs. (12) and (16)}]\). On the other hand, \( \eta = 2 \) holds at high temperatures because there is no long-range order and \( N(Q) \) converges to a constant value \([\text{see Eq. (15)}]\). By contrast, in the intermediate-temperature regime, \( \eta(L, L/2) \) for various \( L \) falls on a single curve. At \( U/V = 1 \), the exponents \( \eta \) at the lower and upper phase boundaries are estimated as \( \eta_{\text{low}} = 0.13(3) \) and \( \eta_{\text{high}} = 0.24(1) \), respectively. These values are consistent with the critical exponents \( \eta_{\text{low}} = 1/9 \) and \( \eta_{\text{high}} = 1/4 \) in the two-dimensional XY model with a \( \Delta_0 \) anisotropy (the six-state clock model). We have numerically confirmed that this result holds true for \( 0 < U < U_c \).

We identify the boundaries of the critical phase as the temperatures where \( \eta \) obtained in the largest system sizes coincides with \( \eta_{\text{low}} = 1/9 \) and \( \eta_{\text{high}} = 1/4 \), and the phase diagram drawn with this criterion is given in Fig. 1.

Note that the equivalent criticality has been suggested in the dislocation-mediated melting in the triangular system \([48]\), the \( J_1-J_2 \) triangular Ising antiferromagnet \([39, 40, 47, 49]\), the triangular Heisenberg model with a single-ion anisotropy \([50, 51]\), the Coulomb crystals in trapped ions \([52]\), and the triangular Blume-Capel model \([53-59]\), which will be investigated further below. In contrast to the Coulomb gas model on a triangular lattice \([60]\), where the BKT transition line hits the first-order transition line slightly below the critical end point, the BKT-like transition lines seem to terminate at a single critical point for all the systems with short-range interactions mentioned above. In general, first-order, second-order, and BKT transitions are allowed in the \( Z_p \) model \((p \geq 5)\), which includes additional interaction terms with relative angles \( 2n\pi/p \) \((n = 2, 3, \ldots, p-2)\) in the \( p \)-state clock model \([61-63]\). The critical bifurcation point at nonzero temperature \( \text{see Fig. 1} \) is inferred to be the Fateev-Zamolodchikov point \([64]\), where the first-order and BKT transition lines terminate \([65-67]\).

FIG. 8. Histogram of the two-component vector \((N_x, N_y)\) for \( U/V = 1 \) for the system size \( N_x = 48 \times 48 \) at (a) \( T/V = 0.325 \), (b) \( T/V = 0.45 \), and (c) \( T/V = 0.7 \).

FIG. 9. Temperature dependence of \( \eta(L, L/2) \) at \( U/V = 1 \) for \( L = 12 \) (crosses), 24 (X marks), 48 (triangles), 96 (circles), and 192 (squares). The horizontal lines indicate the boundary of the critical phase with error bars (shaded areas).
Here $\Delta$, with $S_i = n_i - 1$, the partition function of the extended Hubbard model (see Table II).

Finally, we obtain the Hamiltonian

$$H_{\text{BC}} = \Delta \sum_i S_i^2 + J \sum_{\langle i, j \rangle} S_i S_j - h \sum_i S_i$$

with

$$\Delta = \frac{U}{2} + T \ln 2,$$

$$J = V,$$

and

$$\hbar = \mu - \frac{U}{2} - zV.$$  

Here $\Delta$, $J$, and $z$ denote the strength of single-ion anisotropy, the strength of nearest-neighbor interaction, and the coordination number, respectively. The external magnetic field $h$ takes the place of chemical potential $\mu$ in the extended Hubbard model. The contribution of spin entropy, whose coefficient is proportional to $T$, is now absorbed in the single-ion anisotropy $\Delta$.

Hereafter, we consider the Blume-Capel model with the temperature-independent $\Delta$ at $h = 0$, and compare the properties of this model with those of the extended Hubbard model at half filling. Note that the extended Hubbard model has degeneracy for the spin degrees of freedom which is absent in the Blume-Capel model, and therefore, their finite-temperature phase diagrams are different. The presence or absence of the BKT-like phase can be identified only by calculating the correlation function directly in each model. However, the extended Hubbard model and the Blume-Capel model with $\Delta = U/2$ have essentially the same ground state [see Eq. (21)].

We use the canonical Monte Carlo method [70] in the Blume-Capel model with the conditions similar to those in the extended Hubbard model (see Sec. II B). At sufficiently low temperatures, thermal averaging of the Blume-Capel model $(\langle \cdot \cdot \cdot \rangle_{\text{BC}})$ is essentially the same as that of the extended Hubbard model $(\langle \cdot \cdot \cdot \rangle)$. Consequently, the squared magnetic moment in the Blume-Capel model,

$$M = \frac{1}{N_s} \sum_i \langle S_i^2 \rangle_{\text{BC}},$$

is related to the density of doubly occupied sites $\rho_2$ in the extended Hubbard model by $M = 2\rho_2$ at low temperatures since $\rho_0 = \rho_2$ (see Sec. III C). Instead of the charge structure factor in the extended Hubbard model, we calculate the spin structure factor defined by

$$S(q) = \frac{1}{N_s} \sum_{i,j} \langle S_i S_j \rangle_{\text{BC}} e^{i\mathbf{q} \cdot (\mathbf{r}_i - \mathbf{r}_j)}$$

in the Blume-Capel model. The phase boundaries are determined by the critical exponent $\eta$, which can be estimated by the size dependence of the largest $S(q)$. Hereafter, we choose $J$ as the unit of energy in the Blume-Capel model.

G. Comparisons with the properties of the Blume-Capel model

We compare the phase diagram of the extended Hubbard model (Fig. 1) with that of the Blume-Capel model (Fig. 10). The ground state shows an $\uparrow\downarrow\downarrow$-type three-sublattice magnetic long-range order [53, 55] for $0 < \Delta/J < 1.5$. At $\Delta = 0$, the ground state has quasi-long-range order [58, 70–72]. The first-order transition line bifurcates at the critical end point $(\Delta_c/J, T_c/J) = (1.45(5), 0.38(2))$ into the two boundaries of the critical phase as in the extended Hubbard model. This result suggests that the electron spin degrees of freedom are irrelevant for the stability of the charge BKT-like phase. Note that in a previous study [57] the critical phase was overestimated because the upper boundary was determined by the temperature at which the specific heat takes a maximum value, which is usually higher than the boundary of the critical phase [see Fig. 3(b)].

Although qualitative behavior of the two phase diagrams is similar, the spin degrees of freedom significantly

| $n_i$ | 0 | $\uparrow$ | $\downarrow$ | 2 |
|---|---|---|---|---|
| Degeneracy of $n_i$ | 1 | 1 | 1 | 1 |
| $S_i = n_i - 1$ | $-1$ | 0 | 1 |
| Degeneracy of $S_i$ | 1 | 2 | 1 |

TABLE II. Degeneracy of $n_i$ in the extended Hubbard model and that of $S_i$ in the Blume-Capel model.
FIG. 10. Phase diagram of the Blume-Capel model obtained by Monte Carlo calculations. The first-order transition line (double line) and the two BKT-like transition lines (single lines) merge at the critical point (open circle). The long-range ordered phase is characterized by the \( \uparrow - \downarrow \) spin configuration. Up- and down-pointing triangles denote the upper and lower critical temperatures determined by the points at which the exponents \( \eta \) obtained in the largest system sizes coincide with \( \eta_{\text{low}} = 1/9 \) and \( \eta_{\text{high}} = 1/4 \), respectively. Squares on a dotted line indicate the temperatures at which \( \eta \) starts to depend on system sizes. This exponent \( \eta_{\text{high}} \) estimated similarly to \( \eta_{\text{high}} \) in Fig. 9 by finite-size scaling seems to exceed the expected one \( \eta_{\text{clock}} = 1/4 \) for \( \Delta/J < 0.5 \) within the system sizes we have studied. However, such a behavior for \( \Delta < T \ln 2 \), which corresponds to \( U < 0 \) in Eq. (21), does not appear in the phase diagram for \( U > 0 \) (Fig. 1).

IV. DISCUSSIONS

A. Stability of the charge critical phase

So far, we have considered the possible charge critical phase in the ideal limit. However, the phase could be susceptible to external perturbations. Here we discuss how the charge critical phase and signatures of it survive in such cases.

First, the present critical phase appears at nonzero temperatures, and therefore, external perturbations that would alter the ground state do not necessarily destroy the critical phase. Second, perturbations smaller than thermal fluctuations should be irrelevant to realize the critical phase. Even in the presence of quantum fluctuations, the charge critical phase is expected to survive if the transfer hopping \( t \) or the spin exchange interaction \( J \sim t^2/U \) is sufficiently smaller than the energy scale of temperature \( T \). Furthermore, similar arguments hold for the small perturbations, such as weak long-range or anisotropic Coulomb interactions, small doping, and small bond or site randomness. On the other hand, degeneracy plays an important role in the present critical phase. If the perturbations substantially destroy the degeneracy at very low temperatures by which the system cannot be regarded as the effective \( p \)-state clock model [46] with \( p \geq 5 \), the critical phase may disappear.

The situation would be much more complex when quantum fluctuations are more dominant than thermal fluctuations. At very low temperatures, it is not so obvious whether quantum fluctuations weaken or stabilize the charge critical insulating phase, if any. Moreover, the Mott transition is expected when the transfer hopping becomes comparable to or larger than \( U \) and \( V \). The nature of the Mott transition in the Coulomb gas model with the fermionic degrees of freedom was discussed at the level of correlated wave functions in two dimensions in the ground state [73]. However, it is much harder to investigate a microscopic model at low but nonzero temperatures. Accurate determination of the phase boundaries as a function of \( t/V \) and doping concentration will be left for future study.
B. Possibility of the charge critical phase in materials

One promising candidate to realize the critical phase in materials would be organic compounds which form triangular structures [11–22]. Another candidate would be adatoms on semiconductor surfaces [23–27]. Indeed, the 012-type charge-ordered state is observed in Sn/Ge(111) [74]. Both systems can be effectively described by the extended Hubbard model on a triangular lattice, and the Coulomb interactions, including the nonlocal one, are estimated to be much larger than the hopping [26, 75]. When the effects of anisotropy and randomness are not too large and the systems can be controlled to be at half filling, the charge critical phase may be achievable.

It might be useful to first investigate two broad peaks in the specific heat as a function of temperature to detect the charge critical phase. As we have shown in Fig. 3, the BKT-like transitions are not identical to the points where the specific heat shows maxima. However, these will be weak evidence of the charge critical phase. The lower boundary of the BKT-like phase should be located above the lower-temperature peak in the specific heat, and the upper boundary of the BKT-like phase should be located below the higher-temperature peak in the specific heat.

After confirming the approximate transition points, one should take the snapshots of real space charge configuration in the intermediate-temperature region between the charge-ordered and disordered phases. In the charge critical phase, the number of singly occupied sites is decreased since thermal fluctuations generate the 002 or 022 triangles by breaking the 012 one [see Fig. 5(b)].

C. Other BKT-like phases

In the present paper we have investigated the extended Hubbard model on a triangular lattice at half filling in the atomic limit to clarify the nature of the charge BKT-like phase caused by competing short-range Coulomb repulsion. Similar BKT-like critical phases in the discrete degrees of freedom, such as orbital and chirality, as well as charge, are also expected in other lattice systems for different fillings. For instance, based on possible superlattice structures in adsorbed monolayers [76, 77], one can consider the effective extended Hubbard model at appropriate filling, where the ground state shows corresponding charge order. When the given structures have degenerate configurations such that the system can effectively be regarded as the p-state clock model with \( p \geq 5 \) at low temperatures, the BKT-like critical phase would emerge at finite temperatures [46]. This would also hold true for the orbital and chirality degrees of freedom. Searching for the charge, orbital, and chirality BKT-like phases in other models is left for future study.

V. SUMMARY

We numerically showed that the charge BKT-like phase appears in the intermediate-temperature regime between the charge-ordered and disordered phases in the extended Hubbard model on a triangular lattice at half filling in the atomic limit. In contrast to the conventional BKT phase in the Coulomb gas model with the logarithmic long-range interaction, the present BKT-like critical phase is caused only by the on-site and nearest-neighbor Coulomb repulsion. The critical phase originates from sixfold-degenerate charge-ordered ground states which generate an effective six-state clock model. The critical phase is characterized by the algebraic decay of the charge correlation function accompanied by an emergent U(1) symmetry in the effective clock model at intermediate temperatures, and the increase of the density of doubly occupied sites. We also clarified the effect of spin degrees of freedom on the phase diagram by comparing that in the Blume-Capel model which is an effective model only for the charge degrees of freedom.

We believe that the findings shown in the present paper not only serve as a good starting point for understanding the phase diagram in two-dimensional electron systems with geometrical frustration but also open up the possibility of searching for novel finite-temperature critical phases that can evolve from conventional charge-ordered phases in two-dimensional electron systems. Experimental realization of the charge BKT-like critical phase in materials is desired.

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* rkaneko@issp.u-tokyo.ac.jp
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