Critical Analyses of the $q$-State Clock-Like Phase Transition

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This study adopts the Monte Carlo simulation method to investigate a coupled XY model on two-dimensional triangular lattices. The simulation reveals a $q$-state clock-like phase transition in addition to the original XY phase transition. Analyzing the spin histograms exposes that the strong on-site coupling tends to lock the difference between the phase variables of the two XY order parameters and generates an additional phase transition. The novel discrete $q$-state symmetry arising from the coupling term is demonstrated to join the continuous symmetry of the model in this investigation.

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I. INTRODUCTION

There has much research interest in statistical models of phase transitions and critical phenomena in recent decades [1]. In this paper, we will consider models that simultaneously display both continuous and discrete symmetries. Kosterlitz and Thouless [2] have explained that the two-dimensional XY phase transition is not a conventional continuous phase transition, but rather involves the breakage of bound pairs of the topological vortex and antivortex in the system. Although the continuous aspect of phase transition in the XY model has been studied extensively, the Mermin-Wagner [3] theorem does not exclude the possibility of discrete symmetry breaking. We propose a coupled XY model to investigate the competition between the continuous and discrete phase transitions. Physical systems that simultaneously display both discrete and continuous symmetries have received considerable interest [4–12]. The monolayer phase diagrams of $N_2$ and CO molecules are dominated by the commensurate structures on the basal plane of graphite at a temperature, $T_1$.

At a lower temperature ($T_2 < T_1$) the molecules in this commensurate phase may arrange themselves in a herringbone order [7–10]. Three-state Potts-like phase transitions involving herringbone order have been investigated. The XY continuous transition might compete with some discrete transitions in the system. The Ising-like phase transition was taken into account in competing with the Kosterlitz-Thouless transition in a He$^3$ superfluid film [11]. Thus Lee et al. examined the nonuniversal critical behavior in a coupled XY-Ising model [12]. To examine the nature of the XY transition, Jose et al. [13] perturbed the continuous model by a $q$-fold symmetry breaking field to study the KT theory of the spin wave excitations. Minchau and Pelcovits [14] perturbed the XY system by introducing a random uniaxial field, which points in the $\pm x$ directions. They identified an ordered phase with Ising symmetry in a classical XY model at nonzero temperature. They also considered the p-state generalization of the model, and identified an ordered phase with 2p-fold symmetry.

at nonzero temperature. Notably, the classical XY model can be expressed as many forms of the coupled XY model [15–21] and with variation of the temperature or other parameters, two or more successive transitions can occur in the case of a strongly coupled excitation. Jiang et al. [20, 21] studied a coupled XY model based on a Hamiltonian proposed by Bruinsma and Aeppli [22] for smectic liquid crystals. The on-site coupling between the two XY ordering parameters in the proposed model can generate discrete phase transitions, such as Potts transitions [23]. Jiang et al. [24] demonstrated a unique three-state Potts-like discrete transition following the continuous XY transition in the system. Jiang et al. also found two different orderings established simultaneously via a single continuous phase transition in some coupling parameter domain, and using the new phenomena, interpreted the liquid crystal Sm-A to Hex-B transition [25, 26]. Considerable interest exists in the competition between the continuous phase transition and the discrete aspect in two-dimensional XY systems and in smectic liquid crystal layers [27, 28]. A coupled XY model is proposed in this investigation, in which a possible \( q \)-fold disturbance similar to the three-fold one of Jiang et al. is introduced to the on-site coupling. The proposed model reveals that versatile properties and several distinct phase transitions occur. Besides the classical XY transition, a unique \( q \)-state clock transition is generated in the intrinsic XY system.

II. PHYSICAL MODEL AND ANALYSIS

The coupled XY Hamiltonian in this investigation is as follows:

\[
H = -J_1 \sum_{\langle i,j \rangle} \cos(\theta_i - \theta_j) - J_2 \sum_{\langle i,j \rangle} \cos(\varphi_i - \varphi_j) - J_3 \sum_i \cos(\theta_i - q\varphi_i),
\]

where the first and the second terms are the XY models themselves and the coupling term is introduced in the third term. Two angular variables \( \theta_i \) and \( \varphi_i \) are located at each triangular lattice site \( i \). For the experimental importance, it is more realistic to simulate the model on a triangular lattice than on a square lattice. \( \langle i,j \rangle \) represents the nearest-neighbor pairs of sites and denotes the nearest-neighbors’ coupling in the first two terms. The third term shows that the coupling between the two XY order parameters is localized at the same lattice site. The integer number \( q \) of the coupled XY model will decide the coupling form of the two order parameters. It is noted that as the \( \theta \) and \( \phi \) are coupled relatively strongly, the phase transitions are quite interesting. Therefore \( J_3 = 3.1 \) (larger than both \( J_1 \) and \( J_2 \)) is chosen to examine the phenomena in the following studies.

The simple scenario, the case of \( J_1 > J_2 \) (say, \( J_1 = 1.0 \) and \( J_2 = 0.5 \), is explored in this investigation. Employing the standard Monte Carlo technique, we conducted the simulation works on 36 × 36 triangular lattices with periodic boundaries. The heat-capacity data as a function of temperature for various \( q \) were obtained by calculating the energy fluctuation \( C_V = \frac{1}{N T^2} \langle (H^2) - \langle H \rangle^2 \rangle \), as displayed in Figs. 1(a) – 1(d). During the simulation, the angles \( \theta_i \) and \( \phi_i \) are treated as continuous unconstrained variables. 1,000,000 Monte Carlo steps (MCS) are used for each temperature. To ensure thermal equilibrium, the first 200,000 MCS are discarded. There appear two heat-capacity peaks for \( q \leq 4 \), and three
peaks for $q > 4$. This phenomenon shows that the system proceeds through two phase transitions for $q \leq 4$, and passes through three phase transitions for $q > 4$. We show the heat-capacity diagram of the case $q = 4$ in Fig. 1(a), a sharp peak is located at $T = 0.88$ and a broad hump appears around $T = 1.7$. (The temperature is in units of $J_1$ in this study.) The heat-capacity diagrams of $q = 5$, $q = 8$, and $q = 12$ are displayed in Figs. 1(b), 1(c), and 1(d), respectively. All of the figures display a broad hump around $T = 1.7$. In the case of $q = 4$, another sharp peak shows at $T = 0.88$. It is noted that for the cases of $q > 4$, the sharp peak at the lower temperature is divided into two peaks. An extra transition appears and these two peaks constitute a critical transition region. The new peak of the transition further shifts to the lower temperature as the value $q$ increases. For the case of $q = 5$, the peak is located at $T = 0.64$. For the case of $q = 8$, the peak is located at $T = 0.27$. As for the case of $q = 12$, the temperature of the lowest heat-capacity peak approaches zero shown in the figure. Comparing with the smooth heat capacity peak of a KT type transition, these heat capacities peaks are rather singular. They are affected by the strong coupling of the two order parameters. Especially in the case of $q = 3$, the two peaks would combine to transition simultaneously. And the transition belongs to the special universality class in discussing the exponents of the heat capacity and the helicity modulus.

To illustrate the nature of these phase transitions, the spin histograms of the states near the heat-capacity peaks for various values of $q$ are analyzed directly. For the case of $q = 4$, Figs. 2(a) and 2(e) illustrate histograms of the parameters $\theta_i$ and $\phi_i$ at a low temperature $T = 0.1$, we find both $\theta_i$ and $\phi_i$ are accumulative and exhibit a single hump. Raising the temperature to $T = 0.7$, which is below the first phase transition (whereas $T_{C1} = 0.88$), the distributions of both $\theta_i$ and $\phi_i$ still exhibit a single hump, as shown in Figs. 2(b) and 2(f). Notably, $\phi_i$ initiates small satellite peaks. The temperature is raised gradually to $T = 1.0$, which is the temperature between the first and second phase transition, $T_{C2} = 1.7$. Figures 2(c) and 2(g) display the spin distributions of $\theta_i$ and $\phi_i$. Despite the distribution of $\theta_i$ still displaying a single hump, the distribution of $\phi_i$ separates into four distinct peaks with almost equal height in one period $2\pi$ of $\phi_i$ with an equal interval of $2\pi/4$. Further increasing the temperature to above the $T_{C2}$, the spin distributions at $T = 1.8$ are drawn in Figs. 2(d) and 2(h). Both spin distributions of $\theta_i$ and $\phi_i$ were observed to smear out and distribute over all angles equally, such that $\theta$ and $\phi$ both display an isotropic character.

For the case of $q = 5$, the unusual histograms of $\phi_i$ near the heat-capacity peaks are illustrated in Figs. 3(a) – 3(d). The distribution of $\theta_i$ is not shown here because it has a similar evolution to that of the former case of $q = 4$ for various values of $q$. At low temperature $T = 0.1$, the distribution of $\phi_i$ displays a single peak, as shown in Fig. 3(a). At $T = 0.7$, which is the temperature between the first and second transition temperature ($T_{C1} = 0.64$, $T_{C2} = 0.88$) in the critical region, three peaks rather than the original concentrated single peak are shown in Fig. 3(b). Notably, the number of peaks of the distribution of $\phi_i$ increases with increasing temperature. Further increasing the temperature to just above the $T_{C2}$, the distribution of $\phi_i$ separates into five distinct peaks with almost equal height in one period $2\pi$ of $\phi_i$ with equal interval of $2\pi/5$. The spin distribution of
FIG. 1: Heat-capacity (C) versus temperature. The coupling constants are $J_1 = 1.0$, $J_2 = 0.5$, and $J_3 = 3.1$. Figures (a), (b), (c), and (d) display the cases of $q = 4$, 5, 8, and 12, respectively.

$\phi_i$ at $T = 1.0$ is shown in Fig. 3(c). Figure 3(d) displays the spin distributions of $\phi_i$ at $T = 1.8$, which is the temperature just above the third phase transition ($T_{C3} = 1.7$). The spin distribution of $\phi_i$ is smeared out and spread over all angles equally. For the case of $q = 8$, the distribution evolution of $\phi_i$ is similar to the case of $q = 5$, as shown in Figs. 3(e)
FIG. 2: Histograms for parameters $\theta_i$ and $\phi_i$ of the case $q = 4$. The coupling constants are $J_1 = 1.0$, $J_2 = 0.5$, and $J_3 = 3.1$. Figures (a), (b), (c), and (d) record $\theta_i$, and figures (e), (f), (g), and (h) record $\phi_i$ at $T = 0.1 (< T_{C1})$, $T = 0.7 (< T_{C1})$, $T = 1.0 (> T_{C1})$, and $T = 1.8 (> T_{C3})$, respectively.

For the case of $q = 12$, at $T = 0.1$, in the spin distribution of $\phi_i$ appears three peaks as shown in Fig. 3(i). The first transition temperature is supposed to be lower than $T = 0.1$. The distribution evolution of $\phi_i$ near the other transition temperature is similar to the cases of $q \geq 5$. As shown in the Fig. 3(j), the distribution of $\phi_i$ reveals nine peaks at $T = 0.7$, which is below $T_{C2}$ ($T_{C2} = 0.88$). And at $T = 1.0$, Fig. 3(k) shows that the distribution of $\phi_i$ separates into twelve distinct peaks with almost equal height in one period $2\pi$ of $\phi_i$ with equal interval of $2\pi/12$. At $T = 1.8$, higher than $T_{C3}$ ($T_{C3} = 1.7$), the $\phi_i$ order distributes over all orientations, as shown in Fig. 3(l).

The spin histograms at $T = 0.1$, $0.7$, $1.0$, and $1.8$ show that $\theta$ and $\phi$ proceed through several distinct phase transitions. At low temperatures ($T < 0.1$), both $\theta$ and $\phi$ are ordered, and both spin distributions are accumulative. The bond orientational order corresponds to $\theta_i \approx \theta_j$ and $\phi_i \approx \phi_j$. Notably, $\theta_i \approx \phi_j$ also, owing to the strong on-site coupling of $J_3$. At temperatures higher than $T_{C1}$, the $\theta$ order remains unchanged, the $\phi$ order starts the first XY-like phase transition into a multi-fold degenerate state. The coupling resulting from the third term will be unable to guide the orientation of $\phi$ to follow that of $\theta$. Thus, the bond orientation of order parameter $\phi$ evolves into multiple directions corresponding to the equivalent energy minima in this temperature range. For $q \leq 4$, the system passes through
FIG. 3: Histograms of the parameter $\phi_i$. The coupling constants are $J_1 = 1.0$, $J_2 = 0.5$, and $J_3 = 3.1$. Figures (a), (b), (c), and (d) record the parameter $\phi_i$ for the case $q = 5$ at $T = 0.1$, 0.7, 1.0, and 1.8, respectively. Figures (e), (f), (g), and (h) show the parameter $\phi_i$ for the case $q = 8$ at $T = 0.1$, 0.7, 1.0, and 1.8, respectively. Figures (i), (j), (k), and (l) show the parameter $\phi_i$ for the case $q = 12$ at $T = 0.1$, 0.7, 1.0, and 1.8, respectively.

the transition into a steady $q$ folder degenerate state. For $q > 4$, the system goes through the transition into a multi-fold degenerate intermediate state, and more degeneracy occurs as the temperature is increasing. As the temperature is raised to $T > T_{C2}$, the on-site $J_3$ coupling generates $q$ equivalent steady energy minima in one period $2\pi$ of $\phi_i$ with equal interval of $2\pi/q$. The bond orientation of $\phi$ divides into $q$ distinct directions, and the order parameter of $\phi$ proceeds through the second phase transition. The system exhibits $q$
disorder freedom for the $\phi$ parameter in the degenerate energy state. The simulation results are also inspected by use of the energy histograms and the Binder fourth-order cumulant of energy \cite{29}. The analysis does not reveal any signal of the first order phase transition. A $q$-state clock model presented one second-order transition for $q \leq 4$, two KT transitions for $q > 4$ \cite{30}. As the parameter $q$ increases the lower transition temperature approaches zero, leaving one KT transition in the system. The simulation results present characters of discrete symmetry which resemble that of the $q$-state clock model. As the temperature is further raised, the system melts and proceeds through the last XY phase transition. Both $\theta$ and $\phi$ then are melted into a completely disordered phase. The simulation reveals the unique $q$-state clock-like phase transition in addition to the original XY phase transitions. Analyzing the spin histograms exposes that the strong on-site coupling tends to lock the difference between the phase variables between the two XY order parameters and thus generates an additional phase transition.

The finite-size scaling analysis has been employed to further explore the unique $q$-state clock-like phase transition and thus to determine transition temperatures. The order parameter $m_L$ is defined as the quantity

$$\langle m^2_L \rangle = \left\langle \left( \sum_i \cos \theta_i \right)^2 + \left( \sum_i \sin \theta_i \right)^2 \right\rangle.$$  

(1)

For the cases of $q = 4$, 5, and 8, we perform simulations on $L \times L$ triangular lattices with $L = 12, 24, 36, 48, \text{ and } 60$, respectively. The size- and temperature-dependence of $m^2_L$ are shown in Figs. 4(a) – 4(c) for the cases of $q = 4$, 5, and 8, respectively. The magnitude of $m^2_L$ drops sharply at the critical temperature except for the highest critical temperature, which is another kind of phase transition. At a critical point, the thermodynamic quantity can be reduced as having such a scaling power law behavior:

$$m^2_L \propto N^{(1-\eta/d)},$$  

(2)

where $N$ is the size of the lattice and $d = 2$ is the dimension. By use of the least square fitting on various $N$ according to Eq. (2), the temperature-dependent exponent $\eta$ is plotted in Fig. 6. The magnitude of $\eta$ rather sharply drops at the critical points. By fitting the size- and temperature-dependence of $m^2_L$ and $\eta$, we could almost determine the same critical temperatures of the $q$-state clock-like phase transition as that from the heat capacity peaks. At low temperature, the spins are ordered, so that the induced exponent $\eta$ is close to 0. After $T_{C2}$, the order $\phi$ has been distributed at $q$ orientations, so that the induced exponent $\eta$ is away from 1/4 of the KT theory at the following critical points: $T_C = 0.88$ for $q = 4$, $T_{C1} = 0.64$ and $T_{C2} = 0.88$ for $q = 5$, $T_{C1} = 0.27$ and $T_{C2} = 0.88$ for $q = 8$.

In order to illustrate the occurrence of the $q$-state clock-like phase transition, we summarize the simulation data to plot the phase diagram. Figure 5 shows the schematic diagram of the phase transition sequences as a function of the parameter $q$. The solid dots are determined by the peaks of the heat-capacity. The heavy line at $T = 1.7$ denotes the XY isotropic transition in the system. For $q > 4$, the $q$-state intermediate transition
FIG. 4: Order parameter versus temperature. Figures (a), (b), and (c) show the cases $q = 4$, 5, and 8, respectively. The symbols $\triangle$, $+$, $\square$, $\diamond$, and $\times$, represent the data for $L = 12$, 24, 36, 48, and 60, respectively.

at $T = 0.88$ is denoted by the dashed line. The thin line presents the lowest transition temperature. As the parameter $q$ increases, the transition shifts to lower temperatures. The $q$-state clock intermediate phase is located in the grid region between the dashed line and the light line. It is assumed that as the coupling strength is lowered down and the parameter $q$ is sufficient large, the discrete $q$-state clock-like transition of the coupled XY model would evolve back to the original continuous XY transition.
III. DISCUSSION AND CONCLUSIONS

Two successive phase transitions were found in the antiferromagnetic Ising model model. Mekata has proposed that the antiferromagnetic Ising model on a triangular lattice with ferromagnetic next nearest neighbour interaction is closely related to a six-state clock model. By using a Monte Carlo simulation, Fujiki et al. and Takayama et al. have confirmed that the two successive phase transitions belong to the K-T transition, and that the intermediate phase is characterized by a power-law decay of the spin correlation function. With the finite-size scaling method and Monte Carlo renormalization group methods, Miyashita et al. have discussed the critical points of the two successive transitions. Jose et al. also examined the XY model perturbed by the $q$-fold symmetry breaking field to study the KT theory of the vortex-antivortex pairs coexisting with the spin wave excitations. Two successive phase transitions were also found with the $\eta$ values being 1/9 and 1/4 at $T_{C1}$ and $T_{C2}$, respectively, for the case of $q = 6$.

To summarize the results, we examine a unique coupled XY model on two-dimensional...
The phase transition in the model reveals both continuous and discrete symmetries. The system proceeds through two phase transitions for $q \leq 4$, and through three phase transitions for $q > 4$. Analyzing the spin histograms of $\theta_i$ and $\phi_i$ shows that the $\phi$ order parameter precedes the discrete $q$-state clock-like phase transition. As the value $q$ is sufficiently large, the discrete $q$-state clock-like transition would become a continuous XY transition. The occurrence of the unique $q$-state clock-like phase transition in addition to the XY phase transition is due to the coupling term, which tends to lock the difference between the phase variables of the two XY systems. The coupled XY model ascertains that a discrete symmetry arising from the coupling term...
joins to the original continuous symmetries. And the competition of continuous and discrete symmetries is also demonstrated in the investigation.

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References

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