



New Ordered Phases in a Class of Generalized XY Models

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It is well known that the 2D XY model exhibits an unusual infinite order phase transition belonging to the Kosterlitz-Thouless (KT) universality class. Introduction of a nematic coupling into the XY Hamiltonian leads to an additional phase transition in the Ising universality class [D.H. Lee and G. Grinstein, *Phys. Rev. Lett.* **55**, 541 (1985)]. Using a combination of extensive Monte Carlo simulations and finite size scaling, we show that the higher order harmonics lead to a qualitatively different phase diagram, with additional ordered phases originating from the competition between the ferromagnetic and pseudonematic couplings. The new phase transitions belong to the 2D Potts, Ising, or KT universality classes.

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The low-temperature behavior of two dimensional (2D) systems with continuous symmetries is controlled by topological defects, such as vortices and domain walls. Although massless Goldstone excitations, such as spin waves, destroy the long-range order of these systems, a pseudo-long-range order with algebraically decaying correlation functions still remains possible. At low temperatures the topological defects which undermine the pseudo-long-range order are all paired up, while above the critical temperature these defects unbind, leading to exponentially decaying correlation functions and a loss of the pseudo-long-range order. A classical example of such system is the XY model. At low temperature, the topological defects, in the form of integer valued vortices, are all joined in vortex-antivortex pairs, resulting in algebraically decaying spin-spin correlation functions. Above the Kosterlitz-Thouless (KT) critical temperature [1,2], these pairs unbind and the correlation functions decay exponentially.

Unlike in 3D, for 2D systems the arguments based purely on symmetry considerations are not sufficient to fix the universality class of possible phase transitions [3–6], and even in 3D a second order phase transition can be preempted by a first order one [7]. Violations of strong universality are even more common in 2D. Thus, it is possible for systems with the same underlying symmetries and the same coarse-grained Landau-Ginzburg-Wilson Hamiltonian not to belong to the same universality class. It is, therefore, interesting to ask what phase transitions are possible for 2D Hamiltonians invariant under the transformation $\theta \rightarrow \theta + 2\pi$. In this Letter, we will study using extensive Monte Carlo simulations and finite size scaling (FSS) analysis, a large class of generalized XY models which, while preserving the same $\theta \rightarrow \theta + 2\pi$ symmetry, have very complex phase diagrams, with phase transitions belonging to the Ising and Potts universality classes, in addition to the usual KT phase transition. In some of these models, transitions can be understood in terms of new topological defects, such as fractional vortices and domain

walls [8,9]. Apart from the fundamental considerations regarding the connection between symmetry and universality, our purpose is to describe new, previously unnoticed, ordered phases which occur in 2D systems with continuous symmetry.

The model considered here has a mixture of ferromagnetic and nematiclike interactions,

$$H = - \sum_{\langle ij \rangle} [\Delta \cos(\theta_i - \theta_j) + (1 - \Delta) \cos(q\theta_i - q\theta_j)], \quad (1)$$

where the sum is over the nearest neighbors spins on a square lattice, $0 \leq \Delta \leq 1$, and q is a positive integer. The first term is the usual ferromagnetic coupling (XY model), while the second one favors the adjacent spins to have a phase difference of $2k\pi/q$, where $k \leq q$ is an integer. Independent of the value of Δ , the Hamiltonian (1) has the symmetry of the pure XY model, recovered when $\Delta = 1$, and is invariant under rotations $\theta_j \rightarrow \theta_j + 2\pi$. For $\Delta = 0$, we have a purely nematiclike Hamiltonian, which is also invariant under the transformation $\theta_j \rightarrow \theta_j + 2\pi/q$. It is easy to show that in this case there will also be a KT phase transition at exactly the same critical temperature as in the pure XY model. The low-temperature phase for $\Delta = 0$ will, therefore, have a pseudo-long-range nematiclike order. An interesting question concerns the thermodynamics of the model described by Eq. (1) for $0 < \Delta < 1$, where both terms compete.

For $q = 2$, the Hamiltonian, Eq. (1), has been studied by a number of authors [8–13] and the presence of the second term leads to metastable states in which spins have antiparallel orientation. The model has new excitations not present in the $\Delta = 1$ case: half-integer vortices connected by strings (domain walls) [8], across which spins are in antiparallel alignment. At low temperatures, half-integer vortices are bound in pairs of integer vorticity, resulting in a pseudo-long-range ferromagnetic order. If $\Delta < \Delta_{mc}$, as the temperature is raised, the string tension between half-integer vortices vanishes and the system melts into a

nematic phase. On further increase of temperature, the half-integer vortex-antivortex pairs unbind and the system enters a completely disordered paramagnetic phase. As expected, the transition between the nematic and the paramagnetic phases belongs to the KT universality class [14]. Surprisingly, the transition between the two pseudo-long-range ordered phases—nematic and ferromagnetic—is found to be in the Ising universality class [8]. This behavior has been verified with simulations on the square and triangular lattices [11,12]. On the latter, the geometric frustration introduces also a tiny chiral phase above the KT line, but otherwise the phase diagram retains the same topology as on the square lattice [12]. A related model, with a similar phase diagram, was also studied in Ref. [15]. An interesting question is whether, for $q > 2$, the topology of the phase diagram remains unchanged. To answer this, we have explored using extensive Monte Carlo simulations the equilibrium phase diagram of the Hamiltonian (1) with q ranging from 2 to 10. We find that for $q = 2, 3, 4$ the topology of the phase diagram remains the same as for $q = 2$; however, the transition between the pseudoferro-magnetic and pseudonematic phases belongs either to the 3-state Potts ($q = 3$) or to the 2D Ising ($q = 2, 4$) universality class; see Fig. 1(a). For $q \geq 5$, the topology of the phase diagram changes completely and new phases with a pseudolong range order come into existence.

The simulations were performed on a square lattice of linear size L and periodic boundary conditions. Both Metropolis single-flip and the Wolff algorithm [16] were used. In accordance with the symmetry of the Hamiltonian, the possible order parameters are $m_k = L^{-2} |\sum_i \exp(ik\theta_i)|$ where $k = 1, \dots, q$. The corresponding generalized susceptibilities are $\chi_k = \beta L^2 (\langle m_k^2 \rangle - \langle m_k \rangle^2)$ and the Binder cumulants are $U_k = 1 - \langle m_k^4 \rangle / 3 \langle m_k^2 \rangle^2$ [17,18].

If the transition is not KT, the usual FSS can be used to get the critical exponents β , γ , and ν : $m = L^{-\beta/\nu} f(tL^{1/\nu})$ and $\chi = L^{\gamma/\nu} g(tL^{1/\nu})$, where m is the order parameter and χ its susceptibility, f and g are the scaling functions, and $t = T/T_c - 1$ is the reduced temperature. This FSS, however, is not valid at the KT transition for which all of the low-temperature phase is critical and the correlation length and the susceptibility are infinite [2,19]. Nevertheless, it is possible to show that at the KT transition and in the low-temperature phase, the critical exponent ratios are well defined and the order parameter and the generalized susceptibility scale with the size of the system as $m \propto L^{-\beta/\nu}$ and $\chi \propto L^{\gamma/\nu}$. Exactly at the transition, $\beta/\nu = 1/8$ and $\gamma/\nu = 7/4$, which are the same ratios as for the 2D Ising model. However, what distinguishes the KT transition from the Ising one, is the behavior of the order parameter and the susceptibility in the low-temperature phase where they also exhibit FSS, but with nonuniversal critical exponents. Recall that for normal second order phase transition, FSS exists only at the critical point. This difference can be used to distinguish the KT transition from the Ising one.

Figure 1(a) shows the schematic phase diagram for $q = 3$, which is topologically identical to the $q = 2$ case. At high temperatures, the equilibrium state is the disordered paramagnetic (P). As the temperature is lowered, the system enters either the usual ferromagnetic (UF) or the generalized-nematic phase (N), depending on the value of Δ . Both of these order-disorder transitions belong to the KT universality class. Up to the multicritical point located at $\Delta_{mc} \simeq 0.4$, there is a line of critical points separating the generalized-nematic from the UF phase. The order parameter m_1 is used to distinguish between the generalized-nematic and the ferromagnetic phases: $m_1 \simeq 0$ in the nematic phase and is $\simeq 1$ in the ferromagnetic phase.

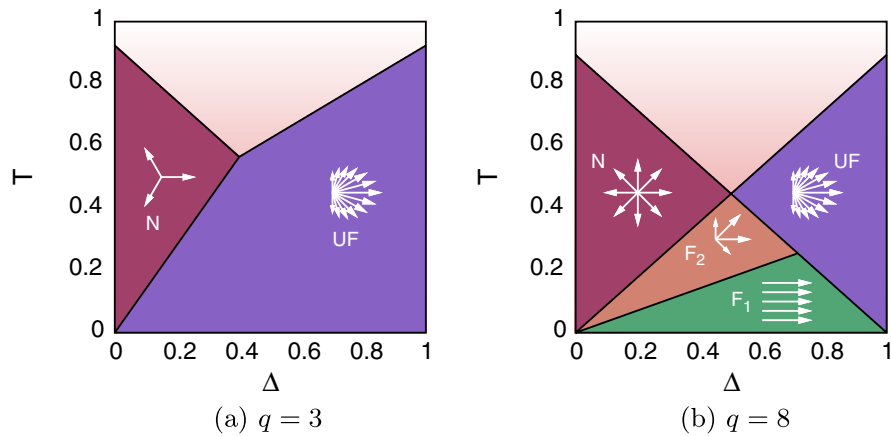


FIG. 1 (color online). (a) Schematic phase diagram for $q = 3$. At both extremes $\Delta = 0$ and 1 , the order-disorder transition temperature is $T_c = 0.893$. There are two low-temperature phases with a pseudolong range order: generalized-nematic (three preferred spin orientations) and ferromagnetic (broken reflection symmetry). Notice the multicritical point around $\Delta_{mc} \simeq 0.4$. For $\Delta < \Delta_{mc}$, there are two transitions: paramagnetic to nematic, in the KT universality class; and nematic to ferromagnetic, in the $q = 3$ Potts universality class. (b) Schematic phase diagram for $q = 8$. Besides the paramagnetic, the usual ferromagnetic, and the nematic phases, there are two new ferromagnetic phases (F_1 and F_2) in which spins have half-plane preferred orientations.

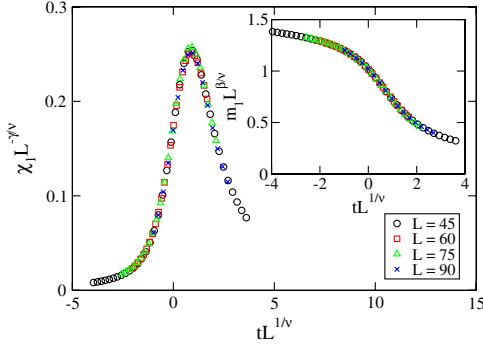


FIG. 2 (color online). Ferromagnetic-nematic transition for $q = 3$. FSS analysis of the susceptibility χ_1 and the order parameter m_1 (inset) for $\Delta = 0.25$ and different sizes L . In both cases the data collapse is excellent using the 3-state Potts exponents. The critical temperature at this point is $T_c \approx 0.365$.

Using FSS, and also the Binder cumulant, we find that the critical points along this line belong to the 3-state Potts universality class. Figure 2 shows the data collapse of m_1 (inset) and the corresponding susceptibility χ_1 , for a critical point with $\Delta = 0.25$. The collapse is excellent using the critical exponents of the 2D, 3-state Potts model [20]: $\beta = 1/9$, $\gamma = 13/9$ and $\nu = 5/6$.

The same topology of the phase diagram persists for $q = 4$, except that the transition from the generalized-nematic to the ferromagnetic phase is once again in the universality class of the Ising model [21,22]. For $q \geq 5$, however, the topology changes dramatically. Two new phases emerge from the $T = 0$, $\Delta = 0$ fixed point; see Fig. 1(b). The new phases are pseudoferrimagnetic and have a broken reflection symmetry. We shall denote these phases as F_1 and F_2 . The low-temperature phase F_1 has only one preferred spin orientation, while in the phase F_2 there are four preferred spin orientations with different weights; see Figs. 1(b) and 4. Figure 4 exhibits histograms of spin orientation in the low-temperature phases along the line $T = 0.16$ together with a pictorial representation of the possible spin orientations for the $q = 8$ model. All the ferromagnetic phases have a quasi-long-range order and a broken reflection symmetry. For F_2 , the distribution function has four significant peaks, while for F_1 there is only a single narrow peak. The UF phase of the XY model has a broad continuous distribution of spin orientations. The nematic phase is characterized by eight congruent discrete spin orientations, separated by $\pi/4$.

Besides the order-disorder KT transitions, several new order-order transition lines appear in the $q \geq 5$ phase diagrams; Fig. 1(b). The transition from the F_1 to F_2 phase is well described by the m_4 order parameter, which is close to zero in the later phase. The data collapse for several lattice sizes is shown in Fig. 3 along with the data collapse for the susceptibility χ_4 . Both collapses were obtained using the set of critical exponents of 2D Ising model: $\gamma = 7/4$, $\nu = 1$ and $\beta = 1/8$. The transition

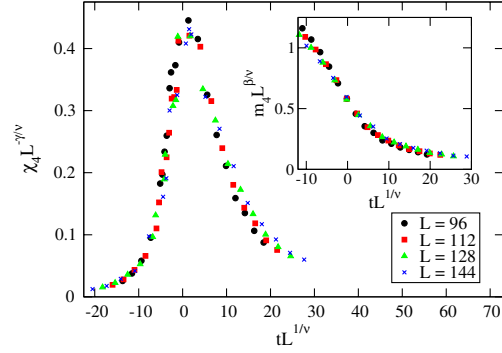


FIG. 3 (color online). Data collapse for the susceptibility χ_4 and the order parameter m_4 (inset) for $q = 8$ at $\Delta = 0.15$ as the system crosses the border between F_1 and F_2 phases. The collapse was obtained using the critical exponents of the 2D Ising model, $\gamma = 7/4$, $\nu = 1$, $\beta = 1/8$, and $T_c \approx 0.058$.

from F_2 to nematic is also continuous and is also in 2D Ising universality class, as can be seen in Fig. 5 in which the data collapse of the order parameter and the corresponding susceptibility are shown. For this transition, the relevant order parameter is m_1 . Finally, the transition from F_1 to UF and the transition from F_2 to UF are both well described by the m_8 order parameter. The two transitions are found to belong to the KT universality class with the critical exponent ratios, $\gamma/\nu = 7/4$ and $\beta/\nu = 1/8$. As an example, Fig. 6 shows that F_2 is critical with respect to m_8 order parameter and has a nonuniversal FSS characteristic of a low-temperature KT phase, top-most curve of Fig. 6.

To conclude, we have studied, using extensive numerical simulations, phase diagrams of a class of generalized XY models described by Eq. (1). Previous results show that for $q = 2$ besides the usual KT transition, there is also a nematic to ferromagnetic transition in the Ising universality class. We find that for $q = 3$ and 4 the topology of the phase diagram remains unchanged, but the ferromagnetic-generalized-nematic transition belongs to the universality

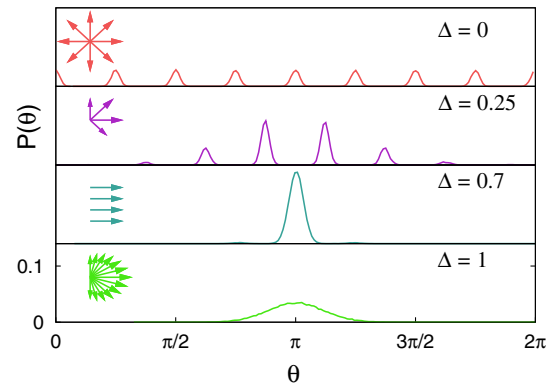


FIG. 4 (color online). Angle distribution for the four phases along the fixed temperature line $T = 0.16$ of the $q = 8$ phase diagram. All graphs have the same vertical scale.

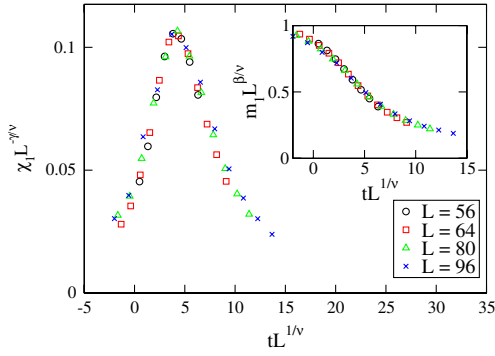


FIG. 5 (color online). Data collapse for the susceptibility χ_1 and the order parameter m_1 (inset) for $q = 8$ at $\Delta = 0.35$ as the system crosses the border between the generalized-nematic and F_2 phases at $T_c \approx 0.34$. The collapse was obtained using the 2D Ising model critical exponents, $\gamma = 7/4$, $\nu = 1$ and $\beta = 1/8$.

class of 3-state Potts and the Ising model, respectively. For $q = 5$, the topology of the phase diagram changes dramatically and two new ferromagnetic phases appear. After this, up to $q = 10$, the maximum value explored in this work, the topology of the phase diagram remains unchanged. It is very curious that although the systems studied here are invariant under the continuous global symmetry $\theta_i \rightarrow \theta_i + \alpha$ (for all spins simultaneously), for arbitrary α , the sequence of the phase transitions between the pseudo-ordered phases follow the one observed for the discrete clock models: $q = 2$ Ising; $q = 3$ Potts; $q = 4$ Ising; for $q = 5$ a bifurcation and a new phase transition appears [23]. If this analogy persists, we expect that there should be a critical value of q above which the phase transition between F_1 and F_2 becomes KT [24]. This will be explored in a future work. The present Letter also shows a significant lack of universality of 2D systems: while all the Hamiltonians studied in this Letter have the same underlying symmetry, $\theta \rightarrow \theta + 2\pi$, the transitions between the

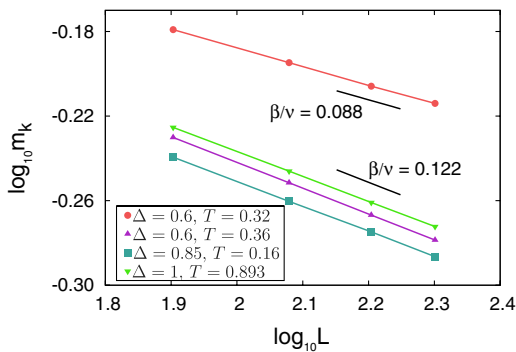


FIG. 6 (color online). Scaling of the order parameter at the KT phase boundaries (three bottommost lines) and inside the critical phase (top-most line) for $q = 8$. Notice that along the KT transition the exponent β/ν has the Ising value ($1/8$), while inside the critical phase the exponent is nonuniversal.

different phases belong to a variety of universality classes. Furthermore, since the Hamiltonians discussed in this Letter can be thought of as the leading orders in a Fourier expansion of a general microscopic spin-spin interaction $V(\theta_i - \theta_j)$, the work raises a troubling question: How much can we really deduce about the thermodynamics of 2D systems from the form of their coarsegrained Landau-Ginzburg-Wilson (LGW) Hamiltonian? It is clear that the symmetry arguments alone are not sufficient to determine the phase diagram of these systems, and one needs to have a detailed knowledge of the microscopic interactions [6].

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