Critical behavior of pure and diluted XY models with uniform frustrations

M. Y. Choi and D. Stroud
Department of Physics, The Ohio State University, Columbus, Ohio 43210
(Received 12 June 1985)

A renormalization-group approach is used to investigate phase transitions in fully frustrated XY models on a square and a triangular lattice. The existence of long-range order associated with the discrete symmetry of the system is demonstrated. It is argued that there exists one transition which is a combination of a Kosterlitz-Thouless—like one for spins and an Ising-like one for chirality. In particular a nonuniversal jump in the helicity modulus is predicted. Dilute randomness is also considered and shown to be irrelevant to the critical behavior.

Since a continuous symmetry cannot be broken in two dimensions,[1] the conventional two-dimensional XY model cannot exhibit long-range order at finite temperatures. Instead, it exhibits algebraic order at low temperatures, which is characterized by a power-law decay of spin-spin correlations. At a certain critical temperature it shows the Kosterlitz-Thouless (KT) transition from this low-temperature algebraic phase to a high-temperature paramagnetic phase.[2,3]

The frustrated XY model, on the other hand, is expected to display different critical behavior since it possesses a discrete symmetry in addition to the underlying continuous $U(1)$ symmetry.[4] Then there can exist two types of topological excitations, vortices (point defects) and domain walls (line defects), leading to the possibility of long-range order in two dimensions.

The observation has created much interest in the two-dimensional XY model, which can be realized by the two-dimensional periodic array of coupled Josephson junctions in a magnetic field.[5–7] The nature of the transition is, however, far from conclusive despite a number of works including Monte Carlo simulations and mean-field calculations. Since fluctuations, in general, play a crucial role in two dimensions, the mean-field approximations are not expected to predict a detailed picture, and a more precise approach is necessary to get a better understanding.

In this work we use a KT-like renormalization-group approach to investigate the critical behavior of fully frustrated XY models on a square and a triangular lattice, and obtain results consistent with available Monte Carlo data. In particular, at low temperatures the system exhibits both algebraic order and long-range order associated with the continuous and discrete symmetry it possesses. As the temperature is increased, both types of excitations condense at a certain critical temperature, leading to a paramagnetic phase at higher temperatures. Therefore there exists one transition of peculiar type, which can be regarded as a combination of a KT-like transition and an Ising-like transition. It turns out that the former is an unconventional one characterized by a nonuniversal jump in the helicity modulus.[8] We also use the replica method to study the effect of bond dilution, and find it to be irrelevant to the critical property of this system.

The uniformly frustrated XY model is described by the Hamiltonian

$$-\beta H = J \sum_{\langle ij \rangle} \cos(\phi_i - \phi_j - A_{ij}) , \tag{1}$$

where A_{ij} is a bond angle such that the plaquette sum is constant over the whole lattice, $\sum A_{ij} = 2\pi f$. This Hamiltonian with the value $f = \frac{1}{2}$, which corresponds to the fully frustrated system, can be decomposed into two coupled XY Hamiltonians

$$-\beta H = K \sum_{\langle ij \rangle} [\cos(\theta_i^{(1)} - \theta_j^{(1)}) + \cos(\theta_i^{(2)} - \theta_j^{(2)})] + h \sum_i \cos p(\theta_i^{(1)} - \theta_i^{(2)}) , \tag{2}$$

where $p = 2$ (3) for a square (triangular) lattice, and both the effective interaction K and the mode-coupling field h depend on the interaction J in the original Hamiltonian (1).[7,9] The form of Hamiltonian (2) naturally manifests the two types of topological excitations expected for the frustrated system: point defects describing vortices in the spins $\theta^{(1),(2)}$ and line defects describing domain walls between regions of different chirality $n = p(\theta^{(1)} - \theta^{(2)})/2\pi$.

The Hamiltonian (2) has been analyzed for $p = 2$ in the context of the helical XY models to predict two phase transitions, of KT and Ising character, respectively.[10] This, however, is not conclusive because the two types of excitations have been assumed to be independent of each other, which is not true in general.

To proceed further, we consider the renormalization of the Hamiltonian (2) by both vortices and the coupling field. In the standard scheme,[3] the coupling field can be taken into account by introducing integer coupling charges in addition to ordinary vortex charges. Correspondingly, we need two types of fugacity controlling the number of vortices and coupling charges, respectively. Also, it should be noted that although the interaction K in the Hamiltonian (2) initially does not couple the two modes, an off-diagonal coupling will be generated by the renormalization process.

With these in mind we can derive the renormalization-group equations. The detailed procedure is essentially the same as that used by several authors,[11] and will not be repeated here. The resulting scaling equations to the lowest order in the vortex fugacity y and the coupling charge fugacity $\tilde{y}$ are

$$\frac{dK}{dl}=\tfrac{1}{2}\tilde{y}^{\,2}-[K^2+(K-\tilde{K})^2]y^2 ,$$
$$\frac{d\tilde{K}}{dl}=\tilde{y}^{\,2}-\tilde{K}^{\,2}y^2 ,$$
$$\frac{dy}{dl}=(2-\pi K)y , \tag{3}$$
$$\frac{d\tilde{y}}{dl}=(2-p^2/2\pi\tilde{K})\tilde{y} ,$$

where $K-\tilde{K}$ accounts for the off-diagonal coupling between the two modes. Initially $\tilde{K}$ is equal to K since the two modes are not coupled, but it is obvious that $\tilde{K}$ becomes different from K as renormalization proceeds. The coupling charge fugacity $\tilde{y}$ is an increasing function of the coupling field h and is given by $\tilde{y}=p\pi^{1/2}h/2$ for small h.

The scaling equations given by (3) show that the coupling field is irrelevant for $\tilde{K}<p^2/4\pi$, while vortices are irrelevant for $K>2/\pi$. When $p=2$ (square lattice), there is no region where both vortices and the coupling field are irrelevant, and the entire spin-wave fixed line is unstable to either vortices or the coupling field. Then the system is expected to exhibit a phase transition from a low-temperature ordered phase, where the coupling field induces long-range order for chirality in addition to algebraic order for spins, to a high-temperature paramagnetic phase where domain walls and vortices destroy such long-range order and algebraic order, respectively.

To see this explicitly, we consider the correlations of both the XY spin and chirality. It is straightforward to derive the expression

$$\Gamma(r)\equiv\langle e^{i\theta_i^{(1)}}e^{-i\theta_j^{(1)}}\rangle=r^{-\eta} ,$$
$$q(r)\equiv\langle e^{in_i}e^{-in_j}\rangle=r^{-\bar{\eta}} \tag{4}$$

with

$$\eta=(2\pi K_{\text{eff}})^{-1}=[2\pi\tilde{K}(2-\tilde{K}/K)]^{-1} ,$$
$$\bar{\eta}=(p/2\pi)^2(2\pi\tilde{K})^{-1} ,$$

where r is the distance between sites i and j, and the interactions K and $\tilde{K}$ now must be interpreted as those approached at large length scales. Since both K and $\tilde{K}$ approach zero at high temperatures, both η and $\bar{\eta}$ become arbitrarily large. This implies an exponential decay of both correlations, which corresponds to a disordered (paramagnetic) phase. On the other hand, both K and $\tilde{K}$ becomes arbitrarily large at low temperatures, leading to the result than η is finite but $\bar{\eta}=0$. Therefore the spins has the usual algebraic order but the chirality acquires long-range order.

To understand the nature of transition in detail, we need a detailed analysis of the scaling equations (3). Although we are unable to do this, it can be shown that, in case $p=2$, $\tilde{K}$ approaches a value greater than $1/\pi$ at the critical temperature. This indicates the relevance of the coupling field around the critical region. The Migdal-Kadanoff approximation considered in Ref. 7 would then be qualitatively correct. The chirality n_i can have values 0,1 at low temperatures, and its order-disorder transition is expected to be of an Ising type.[7] Thus the overall phase transition would be of such a peculiar type that a KT-like transition for spins and an Ising-like one for chirality are combined.

Expected from this observation are Ising-like exponents for chirality and its fluctuation (chirality susceptibility) and a KT-like behavior of the spin susceptibility. The spin helicity modulus, however, is expected to display a jump perhaps greater than the universal one,[12] since the interaction $J(=\sqrt{2}K_{\text{eff}})$ in the original Hamiltonian (1) will approach a value greater than the universal value $2/\pi$ at the critical temperature even though K_{eff} in general approaches a value less than $2/\pi$. Also the specific heat is dominated by the leading singularity, and is expected to display Ising-like behavior, i.e., $\alpha=0$. These predictions are all in agreement with the results of Monte Carlo simulations.[5]

We now consider the case $p=3$ (triangular lattice). At first sight it seems that there exist two consecutive transitions: a KT transition at a certain critical temperature and a second transition having KT-like singularities at a lower temperature, since there is a region where both vortices and the coupling field are irrelevant. This, however, is true only when the initial $\tilde{y}$ is sufficiently small. In fact, the initial value of $\tilde{y}$ corresponding to the original Hamiltonian (1) satisfies $\tilde{y}\sim K^6e^{-9/8K}$ and is not sufficiently small.[13] Closer investigation into this case shows that there is no stability region for the spin-wave fixed line, suggesting only one phase transition.[14] Therefore in both cases (square lattice and triangular lattice) the screening effect of domain walls condensed at the critical temperature is large enough for vortex pairs to unbind at the same temperature.

It can be seen again that the coupling field is relevant around the critical region, and the order-disorder transition of the chirality $n_i(=0,1,2)$ is expected to be described by a three-state Potts interaction with one-site and two-site symmetry-breaking fields,[7] which can be expressed in terms of classical spins $S_i\equiv n_i-1=-1,0,1$:

$$-\beta H=\sum_{\langle ij\rangle}[J_1s_is_j+J_2s_i^2s_j^2]-\Delta\sum_i s_i^2 \tag{5}$$

with the relations $J_1/J_2=3$ and $\Delta/J_1=4$. This is the Blume-Emery-Griffiths model, which has been studied quite extensively.[15] Revealed by these studies is a variety of critical behavior, according to the range of the interactions, including Ising transitions and first-order transitions as well as a three-state Potts transition. For the above range of the interactions, an Ising-like transition is expected. Thus it is concluded that the phase transition of a fully frustrated XY model on a triangular lattice is essentially the same as that on a square lattice. This expectation is strongly supported by Monte Carlo simulations of both the Hamiltonian (1) with $f=\frac{1}{2}$,[6] and the antiferromagnetic XY model on triangular lattices,[16] which should belong to the same universality class.

Finally, we consider the effect of quenched bond dilution, where the probability distribution for the interaction is given by

$$P(J_{ij})=(1-p)\delta(J_{ij})+p\delta(J_{ij}-J) . \quad (6)$$

We use the usual replica method to obtain the effective Hamiltonian in the form

$$-\beta H_{\text{eff}}=pJ\sum_{\alpha=1}^{n}\sum_{\langle ij\rangle}\cos(\phi_i^{(\alpha)}-\phi_j^{(\alpha)}-A_{ij}) , \quad (7)$$

where α is a replica index, and it has been noted that higher cumulants are irrelevant. Performing the same renormalization procedure for this dilute system as that for the pure system, we find that replicas do not mix, and obtain the same scaling equations as those for the pure system, Eq. (3). Thus bond dilution does not affect the critical behavior of the fully frustrated XY model in two dimensions. This result is not surprising since it is known that dilute randomness does not change the critical exponents of the two-dimensional Ising transition.[17]

In summary, we have used the renormalization-group analysis to study phase transitions in the fully frustrated XY models on a square and a triangular lattice, and found novel behavior. The existence of long-range order associated with the discrete symmetry of the system has been demonstrated. It turns out that there exists one transition which is a combination of a KT-like one and an Ising-like one. In particular, a nonuniversal jump in the spin helicity modulus has been predicted. Dilute randomness has been also considered, and shown to be irrelevant to the critical behavior.

Note added. After completion of this work, we learned that similar results for the pure models had been obtained by M. Yosefin and E. Domany [Phys. Rev. B 32, 1778

This work was supported in part by the National Science Foundation through the Materials Research Laboratory at the Ohio State University, under Grant No. DMR-81-19368, and in part by the National Science Foundation under Grant No. DMR-84-14257.

[1]N. D. Mermin and H. Wagner, Phys. Rev. Lett. **17**, 1133 (1966).

[2]J. M. Kosterlitz and D. J. Thouless, J. Phys. C **6**, 1181 (1973); J. M. Kosterlitz, *ibid.* **7**, 1046 (1974).

[3]J. V. José, L. P. Kadanoff, S. Kirkpatrick, and D. R. Nelson, Phys. Rev. B **16**, 1217 (1977). For a review, see D. R. Nelson, in *Phase Transitions and Critical Phnomena,* edited by C. Domb and J. L. Lebowitz (Academic, London, 1983), Vol. 7.

[4]J. Villain, J. Phys. C **10**, 1771 (1977); **10**, 4793 (1977).

[5]S. Teitel and C. Jayaprakash, Phys. Rev. B **27**, 598 (1983); Phys. Rev. Lett. **51**, 1999 (1983).

[6]W. Y. Shih and D. Stroud, Phys. Rev. B **28**, 6575 (1983); **30**, 6774 (1984).

[7]M. Y. Choi and S. Doniach, Phys. Rev. B **31**, 4516 (1985); M. Y. Choi and D. Stroud (unpublished).

[8]T. Ohta and D. Hasnow, Phys. Rev. B **20**, 139 (1979).

[9]In Ref. 7 it was suggested that the system $f=\frac{1}{4}$ on a triangular lattice is also described by the effective Hamiltonian (2). However, this is not likely to be valid since a first-order transition has been indicated by Monte Carlo simulations. The existence of a first-order transition in that system would invalidate the assumption made in Ref. 7 when deriving the corresponding Landau-Ginzburg-Wilson Hamiltonian.

[10]T. Garel and S. Doniach, J. Phys. C **13**, L887 (1980). See, also, Y. Okwamoto, J. Phys. Soc. Jpn. **53**, 2613 (1984).

[11]A. P. Young, Phys. Rev. B **19**, 1855 (1979); D. R. Nelson and B. I. Halperin, *ibid.* **21**, 5312 (1980); J. L. Cardy and S. Ostlund, *ibid.* **25**, 6899 (1982).

[12]D. R. Nelson and J. M. Kosterlitz, Phys. Rev. Lett. **39**, 1201 (1977).

[13]Strictly speaking, the scaling equations (3) are restricted to small values of $\tilde{y}$. However, we assume that Eq. (3) can give qualitiatively correct behavior even for rather large $\tilde{y}$. This seems to hold in the case of two-dimensional XY models with symmetry-breaking fields. See Ref. 3.

[14]Similar situation also occurs in liquid-crystal films. See Ref. 11.

[15]M. Blume, V. J. Emery, and R. B. Griffiths, Phys. Rev. A **4**, 1071 (1971); A. N. Berker and M. Wortis, Phys. Rev. B **14**, 4946 (1976); J. Adler, A. Aharony, and J. Oitmaa, J. Phys. A **11**, 963 (1978).

[16]D. H. Lee, J. D. Joannopoulos, J. W. Negele, and D. P. Landau, Phys. Rev. Lett. **52**, 433 (1984). See, also, S. Miyashita and H. Shiba, J. Phys. Soc. Jpn. **53**, 1145 (1984).

[17]See, for example, R. B. Stinchcombe, in *Phase Transitions and Critical Phenomena,* edited by C. Domb and J. L. Lebowitz (Academic, London, 1983), Vol. 7. The detailed form of the singularity, however, depends on the bond dilution in the two-dimensional Ising transition. See V. S. Dotsenko and V. S. Dotsenko, J. Phys. C **15**, 495 (1982); G. Jug, Phys. Rev. Lett. **53**, 9 (1984).