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Phase transtions in frustrated two-dimensional XY models

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We study the fully frustrated XY model on a square lattice with the use of Monte Carlo simulations. We find a phase transition at a finite temperature T_I with the specific-heat data being consistent with a logarithmic divergence. The helicity modulus Υ jumps to zero with a value $\Upsilon/k_BT \gtrsim 2/\pi$ at a $T \lesssim T_I$. The application of frustrated XY models to the behavior of coupled Josephson junction arrays is discussed.

I. INTRODUCTION

The Kosterlitz-Thouless (KT) theory[1] of the phase transition in the two-dimensional (2D) XY model has been applied to many physical systems including superconducting and superfluid films. Experimental situations have been found which seem to agree well with theoretical predictions. Recently, experiments have been performed[2] to look for KT phase transitions in 2D arrays of coupled Josephson junctions in a transverse magnetic field. In order to investigate the nature of such transitions we have considered uniformly frustrated XY models[3,4] which map onto the coupled junction problem. In particular, the fully frustrated case is studied using Monte Carlo simulations.

II. DESCRIPTION OF MODEL

We consider a class of models described by

$$H = -J_0 \sum_{\langle ij \rangle} \cos(\theta_i - \theta_j - \psi_{ij}) \quad , \tag{2.1}$$

where θ_i is the angle of the planar spin at site i of a square lattice, $\langle ij \rangle$ denotes nearest-neighbor pairs, and ψ_{ij} is a bond angle such that the sum around a plaquette

$$\psi_{ij} + \psi_{jk} + \psi_{kl} + \psi_{li} = 2\pi f \tag{2.2}$$

is constant over the entire lattice. The constant f defined by Eq. (2.2) is referred to as the uniform frustration of the model. The partition function is defined by a sum over the spin variables θ_i.

The Hamiltonian in Eq. (2.1) describes an array of Josephson junctions (one junction on each bond of the lattice) in the low capacitance limit. In this case, we identify $\psi_{ij} = 2e/\hbar c \int_i^j \vec{A} \cdot d\vec{l}$, where $\vec{A}$ is the vector potential. Provided the sample size L is small compared to the transverse penetration depth of the lattice $\lambda_\perp$, i.e., $L < \lambda_\perp \propto 1/J_0$, $\vec{A}$ may be taken to be that of a uniform applied transverse field H_0.[5] The uniform frustration f is related to H_0 by

$$f = H_0 a^2/\Phi_0 \quad , \tag{2.3}$$

with $\Phi_0 = hc/2e$ the flux quantum and a the lattice spacing.

The model specified by Eqs. (2.1) and (2.2) is periodic in f with period 1, and in the interval [0,1] has reflection symmetry about $f = \frac{1}{2}$. The case $f = 0$ corresponds to the ordinary "unfrustrated" XY model which has a Kosterlitz-Thouless phase transition. In this Communication we concentrate on the case $f = \frac{1}{2}$ which corresponds to one-half flux quantum per unit cell of the Josephson junction array. This is the fully frustrated XY model studied in the context of spin-glasses.[3]

III. MONTE CARLO CALCULATIONS

We have studied the behavior of Eq. (2.1) with $f = \frac{1}{2}$ on $N \times N$ lattices with periodic boundary conditions using the standard Metropolis algorithm.[6] The average energy per site $\langle u \rangle$, the specific heat per site C, and the helicity modulus Υ were computed as functions of T. Υ was determined with the use of

$$\Upsilon = -\tfrac{1}{2}\langle u \rangle - \frac{J_0}{k_B T N^2} \times \left\langle \left[\sum_{\langle ij \rangle} \sin(\theta_i - \theta_j - \psi_{ij})(\hat{e}_{ij} \cdot \hat{x}) \right]^2 \right\rangle \quad . \tag{3.1}$$

This may be obtained using a straightforward extension of the analysis of Ohta and Jasnow[7] for the $f = 0$ case. Since the helicity modulus is a measure of the phase correlations of the system, we expect the temperature where Υ goes to zero to indicate the onset of a resistive transition in the Josephson junction array.

Lattices with $N = 8$, 12, 16, 22, and 32 were used and our results are shown in Figs. 1 and 2. Data for $N \leqslant 16$ are the results of one or two independent runs averaged over 25 000 to 50 000 passes with 2000 to 5000 initial passes discarded for equilibration. These were sufficient to achieve equilibrium at all temperatures, and obtain statistically independent data.[8] For $N > 16$, however, to circumvent long

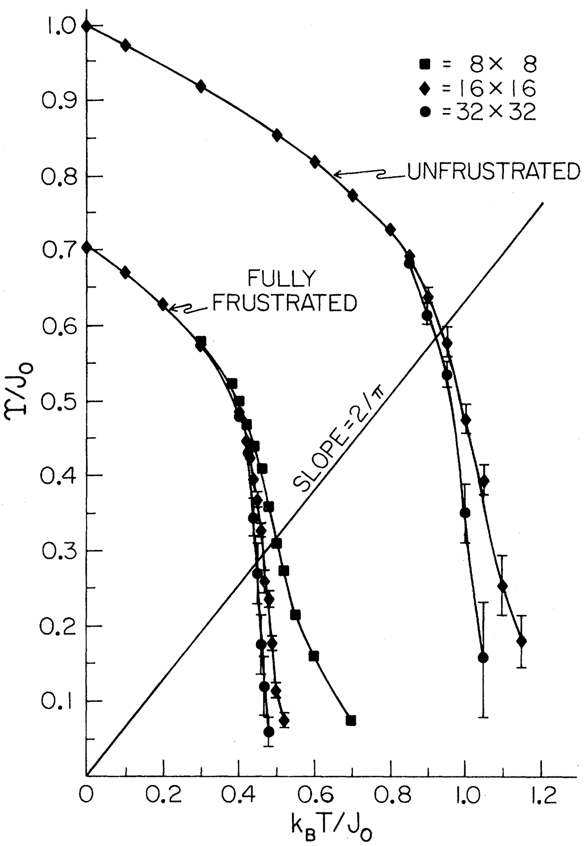

FIG. 1. Helicity modulus Υ vs temperature T for the unfrustrated ($f=0$) and fully frustrated ($f=\frac{1}{2}$) cases, and various lattice sizes N. A line of slope $2/\pi$ indicates the universal jump in $\Upsilon(T_c)/k_BT_c$ of a Kosterlitz-Thouless transition.

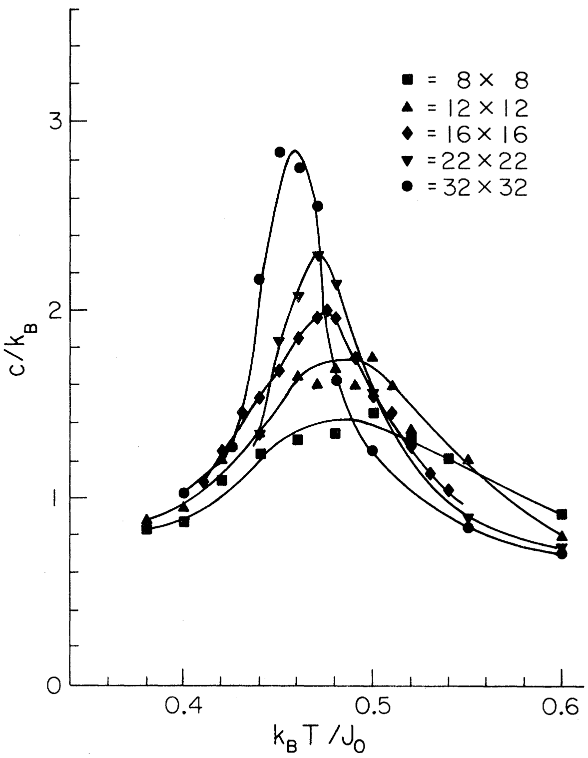

FIG. 2. Specific heat C of the fully frustrated ($f=\frac{1}{2}$) model for various lattice sizes N. The smooth curves through the data are drawn as guides to the eye and are not the result of any theoretical computation.

correlations near T_c, five independent runs, each averaging over 10 000 passes with an initial 5000 discarded, were performed. Our data represent the average of these five runs. Error bars have been estimated by considering the distribution of values obtained when averaged over shorter times.

Our results for $\Upsilon(T)$ are shown in Fig. 1 for the cases $f=\frac{1}{2}$ and $f=0$. The unfrustrated XY model undergoes a KT transition with a universal jump[9] in Υ at $T=T_c$:

$$\lim_{T\to T_c} \Upsilon(T)/k_BT = 2/\pi \quad . \tag{3.2}$$

A line of slope $2/\pi$ is shown in Fig. 1. The $f=0$ results and Eq. (3.2) (finite-size effects have broadened the discontinuous jump) permit an estimate of T_c, $k_BT_c \cong 0.95J_0$ compatible with previous results.[10,11] The low-T behavior $\Upsilon_{f=0} \cong J_0 - k_BT/4$ agrees with the results of Ohta and Jasnow.

Results for the $f=\frac{1}{2}$ case show clear evidence for a phase transition at a finite temperature $k_BT_c \cong 0.45J_0$. $\Upsilon(T)$ goes to zero more steeply than in the unfrustrated cases and is consistent with a jump equal to or perhaps slightly larger than the Nelson-Kosterlitz value (3.2).

In Fig. 2 we exhibit our results for the specific heat per site C computed using the fluctuation-dissipation relation for $f=\frac{1}{2}$ and various lattice sizes N. The peak value of the specific heat $C_{\max}$ is plotted as a function of N in Fig. 3. In marked contrast to the unfrustrated case where $C_{\max}$ saturates at a finite value of about $1.5k_B$,[10,12] we see that $C_{\max}$ increases with N. An exponent of $\alpha=0$(logarithmic) characteristic of an Ising transition is indicated by the linear relation between $C_{\max}$ and $\ln N$. Estimates of $C_{\max}$ obtained by differentiating the computed average energy are consistent with the values obtained from the fluctuation-dissipation relation.

We also note that, whereas in the unfrustrated model the specific-heat peak lies $\sim$10% above T_c,[10,12] the peak for the fully frustrated case lies much closer to the temperature where $\Upsilon\to 0$. Our calculations are not precise enough to distinguish whether $C_{\max}$ occurs at the same temperature as where $\Upsilon\to 0$ or slightly above.

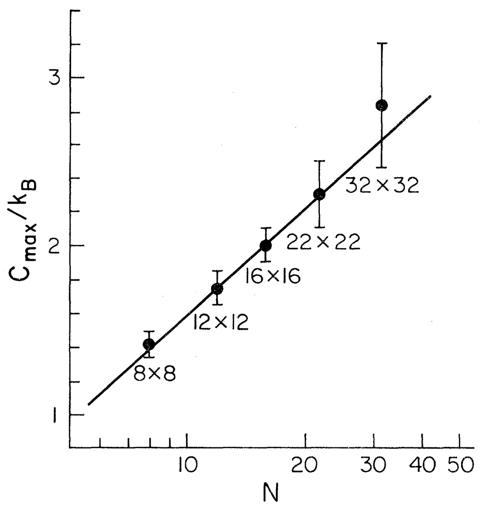

FIG. 3. Maximum specific heat C_{max} vs lattice size N for the fully frustrated ($f=\frac{1}{2}$) case. The linear relation $C_{max} \propto \ln N$ indicates an exponent of $\alpha=0$ (logarithmic divergence).

IV. INTERPRETATION OF RESULTS

In order to interpret the results of the numerical simulations we consider the generalized Villain model believed to be in the same universality class.[13] By using standard duality transformations, the partition function can be separated into a Gaussian spin-wave part and a fractionally charged Coulomb gas with a Hamiltonian,[3,4]

$$H_C = \pi \tilde{J}_0 \sum_{ij} (m_i + f_i) G_{ij} (m_j + f_j) \quad , \tag{4.1}$$

where G_{ij} is the lattice Green's function and the sum is over all sites of the dual lattice; $\tilde{J}_0$ is the coupling of the generalized Villain model, f_i is the frustration of the plaquette around the dual site i and equals the constant f of Eq. (2.2) for our uniformly frustrated model. The m_i's are integer variables. We may define the "charge" at site i, n_i by

$$n_i = m_i + f \quad . \tag{4.2}$$

Averages are evaluated by summing over values of $\{m_i\}$ that lead to neutral ($\sum n_i = 0$) configurations. We see from Eq. (4.1) that the ground state for the $f=\frac{1}{2}$ model consists of an alternating lattice of $n_i = \pm\frac{1}{2}$ charges and is doubly degenerate (corresponding to $n_i \rightarrow -n_i$). If we restrict our attention to $n_i = \pm\frac{1}{2}$, excitations, which must preserve charge neutrality, correspond to rearrangements of the ground-state charges. Identification of $+\frac{1}{2}$ and $-\frac{1}{2}$ charges with up and down spins, respectively, maps our model onto a long-range Ising antiferromagnet with conserved magnetization.[3]

We believe that the two types of excitations illustrated in Fig. 4 are of importance in understanding the numerical results: Type (a), which we call KT-like, results from the interchange of a given $+\frac{1}{2}$, $-\frac{1}{2}$ pair with separation r and has energy proportional to $\ln r$; and type (b), which we call Ising-like, results from the formation of a neutral domain of the other ground state which, in the limit of large domains, has an energy proportional to the perimeter.

The Ising-like excitations, resulting from the twofold degeneracy of the ground state, cause the logarithmic divergence of the specific heat at T_I. The identification with an Ising antiferromagnet suggests a discrete order parameter, the "staggered magnetization" of the n_i (Ref. 14)

$$\mathfrak{N} = \frac{1}{N} \sum_i (-1)^{(\hat{x}\cdot\vec{r}_i + \hat{y}\cdot\vec{r}_i)} n_i \quad . \tag{4.3}$$

To understand the behavior of the helicity modulus Υ, we express it in terms of the dielectric constant of the Coulomb system following Ohta and Jasnow[15]:

$$\Upsilon/\tilde{J}_0 = \epsilon_0^{-1} = 1 - \frac{4\pi^2 \tilde{J}_0}{k_B T} \lim_{k\rightarrow 0} \frac{\langle n_k n_{-k} \rangle}{k^2} \quad . \tag{4.4}$$

Υ is reduced from its $T=0$ value by excitations which develop a net dipole moment, such as the KT-like excitations [Fig. 4(a)] or certain of the Ising-like excitations [Fig. 4(b)].

Noting the identification of Υ with ϵ_0^{-1}, one can repeat the original Kosterlitz-Thouless argument regarding the instability with respect to free charge formation,[16] and deduce the condition

$$\Upsilon(T)/k_B T \geq 2/\pi \quad . \tag{4.5}$$

Thus $\Upsilon(T)$ must drop discontinuously to zero at some temperature T_c with a jump equal to or greater than the universal value $2/\pi$. Two possible scenarios seem likely:

(i) As T_I is approached from below, the Ising excitations result in a steep drop in $\Upsilon(T)$ from its low-T value. As $\Upsilon/k_B T$ approaches $2/\pi$, however, the KT excitations become important, producing a universal

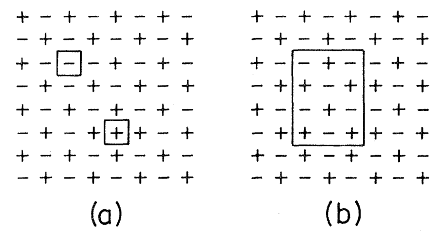

FIG. 4. Two types of excitations of the fully frustrated ($f=\frac{1}{2}$) model; Kosterlitz–Thouless-like (a), and Ising-like (b).

jump $2/\pi$ in $\Upsilon(T)/k_B T$ at some temperature $T_c \leq T_I$.

(ii) As T_I is approached from below, the Ising excitations result in a nonuniversal jump in $\Upsilon/k_B T > 2/\pi$ at the same temperature as the specific-heat peak T_I. Our numerical simulations cannot adequately distinguish between these two possibilities.

V. CONCLUDING REMARKS

Thus we find clear evidence for a phase transition in the $f=\frac{1}{2}$ model. The discrete degeneracy of the ground state of the $f=\frac{1}{2}$ model has played a crucial role in determining the nature of the transition. As f is varied continuously, the charge configuration and the degeneracy of the ground state will vary discontinuously. Thus the system should display interesting properties as a function of f (or external field H_0 in the Josephson junction array). In particular, we have performed calculations of the ground-state energy u_0 for several *rational* f and find that $u_0(f)$ is nonmonotonic in $f \in [0, \frac{1}{2}]$. Since $u_0(f)$ will be proportional to the $T \rightarrow 0$ critical current of the Josephson junction array, such structure should also be observable experimentally. Preliminary calculations of $\Upsilon(T)$ for the $f=\frac{1}{3}$ model indicate a $k_B T_c \approx 0.25 J_0$; thus T_c is also nonmonotonic as a function of f (or H_0). The model in Eq. (2.1) should display a rich variety of phenomena as a function of f which we are currently exploring.

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[14]We have computed $\mathfrak{M}$ in our Monte Carlo simulations by equating the n_i to the vorticity of the phase variables. We find a nonzero $\mathfrak{M}$ at low T, decreasing steeply to zero around T_I.

[15]For the $f=0$ case, Ref. 7 contains a more general formula for Υ in the cosine model of Eq. (2.1). This cannot be applied to the $f=\frac{1}{2}$ model directly since it involves an expansion in the vortex fugacity. The excitations of Fig. 4(b) rule out the possibility of such an expansion. For the Villain model, however, the extension to general f is straightforward. See also, P. Minnhagen and G. G. Warren, Phys. Rev. B 24, 2526 (1981).

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