Two Phase Transitions in the Fully Frustrated XY Model

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The fully frustrated XY model on a square lattice is studied by means of Monte Carlo simulations. A Kosterlitz-Thouless transition is found at $T_{\mathrm{KT}} \approx 0.446$, followed by an ordinary Ising transition at a slightly higher temperature, $T_c \approx 0.452$. The non-Ising exponents reported by others are explained as a failure of finite-size scaling due to the screening length associated with the nearby Kosterlitz-Thouless transition.

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The critical behavior of two-dimensional fully frustrated XY (FFXY) models has been the subject of much interest during the last decade. This is seen in the large number of papers in the literature, of which a number are very recent. In spite of this, the controversy of the nature of the phase transition(s) in these models is by no means settled.

The models under discussion include the antiferromagnetic XY model on a triangular lattice [1,2], the square-lattice version of the XY model with one antiferromagnetic coupling per plaquette [3,4], and the corresponding Coulomb gas with half-integer charges [5,6]. Also discussed in this context are the coupled XY Ising system [7] and the 19-vertex version of the fully frustrated XY model [8], which are believed to be in the same universality class. In the present Letter we focus on the square-lattice version of the FFXY model, but since the results are expected to have a more general validity, we will repeatedly refer to studies of the other above-mentioned models.

Besides the theoretical questions regarding the universality class, the study of the fully frustrated models is largely motivated by their relevance for Josephson junction arrays in a magnetic field. Because of this relation, the Hamiltonian of the FFXY model on a square lattice is customarily written with the vector potential A_{ij},

$$H = -J \sum_{\langle ij \rangle} \cos(\theta_i - \theta_j + A_{ij}) .$$

Here i and j enumerate the lattice sites, θ_i is an angle associated with site i, and the sum is over nearest neighbors. The frustration is determined by the A_{ij}. Full frustration corresponds to one-half flux quantum per plaquette, which means that $f \equiv (1/2\pi) \sum A_{ij} = 1/2$, where the sum is taken around a plaquette; cf. Eq. (3) below.

The ground state for this model on a square lattice [3] has plaquettes with clockwise and counterclockwise rotation in a checkerboard pattern. The angular difference between nearest neighbors is $\phi_{ij} \equiv \theta_i - \theta_j + A_{ij} = \pm\pi/4$. This checkerboard pattern gives rise to the discrete Z_2 symmetry of the antiferromagnetic Ising model, beside the rotational XY symmetry. At low temperatures this model therefore has both the topological long-range order of the XY model, and the ordinary long-range order of the antiferromagnetic Ising model. As the temperature is increased, both the XY-like and Ising-like orders are expected to vanish.

In the first Monte Carlo (MC) study of this model, Teitel and Jayaprakash [4] found a steep drop in the helicity modulus, signaling the loss of XY order, accompanied by an increase in the specific heat with lattice size, consistent with an Ising transition. Being unable to determine the precise critical behavior of the FFXY model, the authors put forward two possible scenarios.

(i) As the Ising temperature, T_c, is approached from below, the Ising excitations produce a steep drop in the helicity modulus. As this quantity approaches the universal value, the Kosterlitz-Thouless (KT) excitations become important producing a universal jump. This occurs before the loss of Ising order, $T_{\mathrm{KT}} < T_c$.

(ii) As T_c is approached from below, the Ising excitations give rise to a jump larger than the universal value [9]. The loss of Ising and XY order take place at the same temperature, $T_{\mathrm{KT}} = T_c$.

Since then, several investigations have been made with the aim to decide between these two possibilities. Whereas some of the earliest MC studies were not decisive [1,2], a large number of recent papers [6–8,10–14] on FFXY models have yielded exponents for the Z_2 transition that differ from the pure Ising ones, suggesting a new universality class, the second possibility above. The evidence is, however, not conclusive, since the finite-size scalings in these papers are not quite satisfactory.

In this Letter we present some MC analyses that shed new light on the behavior of the FFXY models. We first give evidence for an ordinary KT transition. We then demonstrate that the presence of the screening length associated with this transition in the region immediately above T_{KT} precludes the use of ordinary finite-size scaling, and argue that this is the reason for the reported non-Ising exponents. We then determine the Z_2 correlation length, present evidence for an Ising temperature $T_c > T_{\mathrm{KT}}$, and demonstrate that our data are, indeed, consistent with the pure Ising exponent, $\nu = 1$. Our MC data were obtained on a bunch of workstations, by means of the ordinary Metropolis algorithm. The results in the present Letter are in agreement with the suggestion made

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in Ref. [1] on the basis of less conclusive analyses of MC data from a triangular lattice.

The precise determination of the temperature for a Kosterlitz-Thouless transition is a difficult task. This is due to both the absence of spectacular peaks and a logarithmic correction that gives problems with ordinary finite-size scaling. A way to cope with these difficulties, by extracting the finite-size dependence from the Kosterlitz' renormalization group equations, was suggested some years ago [15]. The result may be expressed as a finite-size scaling relation for the helicity modulus [16] valid right at the transition temperature $T_{\rm KT}$,

$$\frac{\Upsilon_L \pi}{2T_{\rm KT}} = 1 + \frac{1}{2(\ln L + l_0)}. \quad (1)$$

Here L is the system size, Υ_L is the helicity modulus for that size, and l_0 is a parameter to be determined. The successful application of this relation does, however, require some care. In the XY model the amplitude of the spin waves change with both temperature and lattice size, which makes it necessary to identify the temperature scale of relevance for the vortices, the Coulomb gas (CG) temperature, $T^{\rm CG}$ [17,18]. In the Coulomb gas this is no problem, but to obtain the equivalent of the helicity modulus one has to include another term in the Hamiltonian containing the polarization squared [19,20]. The data obtained in this way do, indeed, fit very well by Eq. (1) [21].

Figure 1 shows the result from this kind of fit for the FFXY model. Note that the scaling relation is obeyed only for rather large lattices, $L \gtrsim 32$. This is not surprising since Eq. (1) is expected to be valid only for low renormalized vortex density. A KT transition at a low Coulomb gas temperature [6], as in the model under consideration, has to be monitored at larger lengths in order to get data from the region sufficiently close to the critical point. The fit gives $T_{\rm KT}^{\rm CG} = 0.12847(4)$ corresponding to $T_{\rm KT}/J = 0.4460(1)$. We note that this is clearly below $T/J \approx 0.454$, which is a typical value of the Z_2 transition temperature in the literature [11–13].

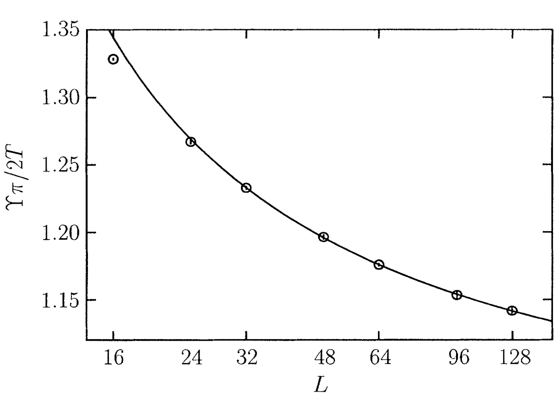

FIG. 1. $\Upsilon\pi/2T$ versus lattice size at $T_{\rm KT}^{\rm CG} = 0.128\,47$ together with the finite-size scaling function, Eq. (1). The good fit is strong evidence for an ordinary KT transition.

For the study of the Z_2 transition it is customary to define the staggered magnetization

$$M = \frac{1}{L^2} \left| \sum_{\mathbf{r}} (-1)^{r_x + r_y} m_{\mathbf{r}} \right|, \quad (2)$$

where the sum is over all the plaquettes of the system, and m is the vorticity. We define the vorticity, in terms of the rotation of the current $\sin\phi_{ij} \equiv \sin(\theta_i - \theta_j + A_{ij})$ around a plaquette [1],

$$m = \frac{1}{\sqrt{8}} (\sin\phi_{12} + \sin\phi_{23} + \sin\phi_{34} + \sin\phi_{41}). \quad (3)$$

The normalization factor in Eq. (3) is chosen from the zero-temperature value of m, which follows from the angular difference $\phi = \pm\pi/4$ in the ground state.

Several recent MC analyses of the Z_2 transition in the FFXY models make use of the expected finite-size dependence of various quantities at criticality [6–8,10–13]. Such methods have generally yielded non-Ising exponents, suggesting a single transition in a new universality class. One of several different approaches is to make use of properties of the distribution function of M at criticality. This has been done both directly in the FFXY model [13] and in the corresponding Coulomb gas [6].

The tacit assumption behind these scaling analyses is, however, that the system size is the only relevant length at criticality. The presence of a nearby transition with a corresponding characteristic length, λ, may well invalidate this assumption. This therefore calls in question the attempts to determine the critical exponents of the Z_2 transition in the FFXY models by finite-size scaling at T_c. The condition for a successful application of finite-size scaling would be $L \gg \lambda$, which may imply prohibitively large lattices.

The effect of this additional length is clearly seen in the dependence of M on the boundary conditions (BC). Beside the ordinary periodic BC (PBC) we make use of fluctuating BC (FBC) [22] obtained by introducing phase mismatches across the boundaries in the x and y directions as a pair of additional dynamical variables. It is with these BC that the XY model corresponds to the CG with periodic BC [5,20,22]. Results for the magnetization obtained with these two BC, and $L = 16$, 64, are shown in Fig. 2. As the figure shows, there is a size-dependent temperature region where M is sensitive to the BC. A comparison with the helicity modulus (dashed lines) shows that the difference between the two curves vanishes when $\Upsilon_L \approx 0$. This condition implies $L \gg \lambda$ since the vanishing of Υ means that vortex pairs at distance $\approx L$ are free.

The dependence of M on the BC is presumably a reflection of the dependence of the vortex interaction on the BC [20], an effect that vanishes if $\Upsilon = 0$. The conclusion from this figure is therefore that the value of

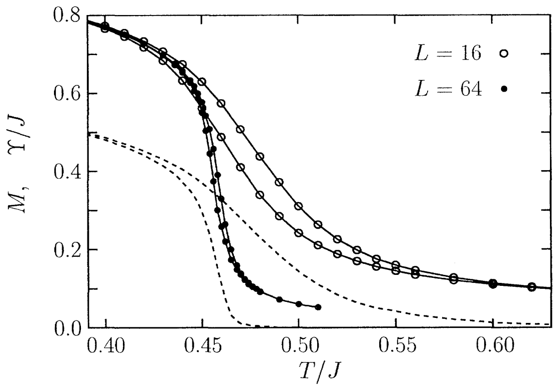

FIG. 2. Staggered magnetization, M, with different BC. Data for PBC lie above the corresponding data for FBC. The dashed lines are the helicity modulus for the same sizes. The data differ at temperatures where $\Upsilon \neq 0$.

M, at fixed T, is uniquely determined by the system size, only if $L \gg \lambda$.

The implications for ordinary finite-size scaling is illustrated with Binder's cumulant [23],

$$U = 1 - \frac{\langle M^4 \rangle}{3\langle M^2 \rangle^2}.$$

For the usual cases where finite-size scaling works, this quantity is size independent at the critical point, $U_L = U^*$. Both the critical temperature and the exponent ν are then obtained from the crossing of U_L for different L. Figure 3 shows this kind of analysis for the FF*XY* model with both PBC and FBC, upper and lower points, respectively. A determination of T_c from data obtained with PBC, would give $T_c \approx 0.454J$, in agreement with previous results [11–13]. Nearly the same critical temperature is obtained from the data obtained with FBC. In both cases there is, however, no unique crossing point independent of the lattice sizes.

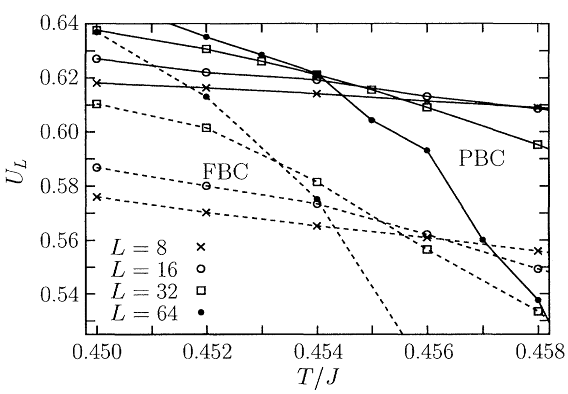

FIG. 3. Binders cumulant as a function of temperature for the two different BC and several lattice sizes. The difference between data from PBC and FBC (solid and dashed lines, respectively) casts doubt on the results from this kind of analysis.

Besides the lack of a unique crossing point, the problem with this kind of analysis is that data for the two different BC suggest different values of U^*. It is, however, clear that there can be only one correct value for U^*. This follows since U_L for sufficiently large L will be independent of the BC.

Our conclusions so far for the Z_2 transition are, firstly, that the reported non-Ising exponents are artifacts due to the screening length that invalidates the scaling assumption, and, secondly, that in order to obtain reliable data for the analysis of the Z_2 transition one has to make use of systems with $L \gg \lambda$, or, equivalently, $\Upsilon \approx 0$.

For the determination of the Z_2 correlation lengths around T_c, we introduce the correlation function

$$g(\mathbf{r}) = (-1)^{r_x + r_y} \langle m_0 m_{\mathbf{r}} \rangle, \tag{4}$$

where the prefactor takes care of the antiferromagnetic structure.

Below T_c this function decays to a finite value in the large-r limit, $g(r) \to M^2$. The decay to this constant is governed by the correlation length ξ_-,

$$g(r) - M^2 \sim e^{-r/\xi_-}. \tag{5}$$

Figure 4 shows $g(r)$ at T_{KT}. The data are for both PBC and FBC, at lattices of size $L = 64, 128$. From the experience with these BC [22] we expect $g(r)$ for an infinite system to lie in between the values for the largest lattices. The solid line in Fig. 4 is from Eq. (5) with $M^2 = 0.376$ and $\xi_- = 6.1$, giving strong evidence that the Z_2 transition takes place at a higher temperature, $T_c > T_{\mathrm{KT}}$.

Granted the existence of two separate transitions, one certainly expects the pure Ising exponents for the Z_2 transition. To verify that expectation by MC simulations, we turn to the temperature dependence of the correlation length above T_c. In that temperature region M vanishes, and the correlation function $g(r)$ behaves as

$$g(r) \sim e^{-r/\xi}. \tag{6}$$

Again, we make use of data for lattices and temperatures such that $\Upsilon \approx 0$, which also turns out to be a prerequisite

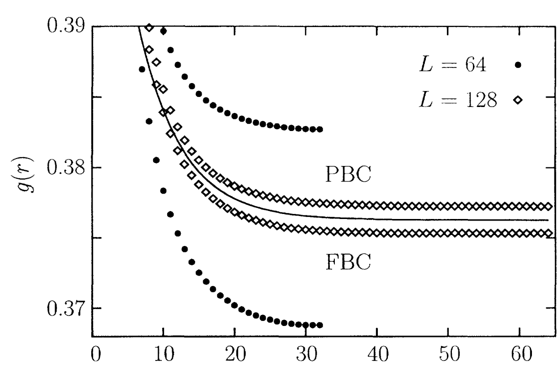

FIG. 4. Correlation function at T_{KT}. Data are for PBC and FBC, upper and lower points. The finite values at large r shows that this temperature is below T_c.

for a good fit to Eq. (6). This means that we are only able to obtain reliable values for ξ at temperatures down to $T/J = 0.472$. As an additional complication, we also have to consider effects from the temperature dependence of the spin waves.

The effect of the spin waves on the behavior of the FFXY model seems to be overlooked so far. In the analysis of the Z_2 transition, the importance of the spin waves stems from the fact that the energy associated with a domain wall becomes smaller with larger spin wave amplitude. There are two possible contributions to the temperature dependence: The average value of $|m|$ for a single plaquette changes with temperature, and the bare vortex interaction may be affected by the spin waves.

To appreciate the significance of this effect one may well compare with an Ising model, $H_I = -K\sum_{\langle ij\rangle} s_i s_j$, with nonsingular temperature dependences in both the coupling constant and the magnitude of the spins. In the immediate vicinity of T_c these temperature dependences may be neglected with impunity, but with data in a larger temperature region, one has to resort to an effective temperature variable, $T^I = T/Ks^2$. To apply this kind of reasoning to the FFXY model we suggest making use of the expression for the bare vortex interaction from Ref. [20]. With m defined as in Eq. (3), the energy associated with the vorticity at the origin and $\mathbf{r}$ becomes

$$E_{\text{bare}}(\mathbf{r}) = \frac{8J^2}{J_0} m_0 G(\mathbf{r}) m_{\mathbf{r}}\,,$$

where $J_0 = J\langle\cos\phi\rangle$. This suggests that the relevant temperature scale is

$$T^I = \frac{T}{\langle|m|\rangle^2 J/J_0}\,.$$

Figure 5 shows $1/\xi$ plotted against T^I. This is a demonstration that the temperature dependence of ξ is, indeed, consistent with the pure Ising exponent, $\nu = 1$.

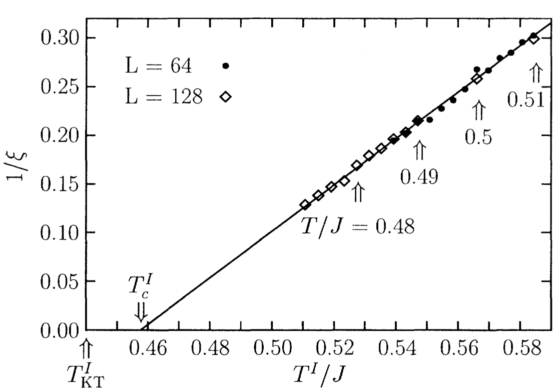

FIG. 5. The dependence of the Z_2 correlation length on the effective temperature. With $\xi^{-1/\nu} \propto T^I - T_c^I$, the data are consistent with the pure Ising exponent $\nu = 1$.

The analysis also suggests a value of the Ising temperature. The figure gives $T_c^I/J = 0.4576(13)$, slightly above $T_{\text{KT}}^I/J \approx 0.440$. In ordinary temperatures this corresponds to $T_c/J = 0.452(1)$, which is consistent both with T_{KT} as a lower bound and the crossing points in Fig. 3 as upper bounds for T_c.

In conclusion, we have found ample evidence for two distinct transitions in the FFXY model on a square lattice. The KT transition is analyzed by finite-size scaling of the helicity modulus, the previously obtained non-Ising exponents are explained as a failure of the scaling assumption, and, with the identification of the relevant temperature scale, the data are consistent with the Ising exponent, $\nu = 1$.

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