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Monte Carlo study of frustrated *XY* models on a triangular and square lattice

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The critical behavior of the fully frustrated *XY* model on a triangular and square lattice is investigated by Monte Carlo simulations. From a finite-size-scaling analysis, we determine the critical exponents associated with the chirality order parameter. Contrary to previous simulations, we find the exponents to be inconsistent with the pure Ising values. We argue that these results are in favor of a single transition in a new universality class.

Fully frustrated *XY* (*FFXY*) models were introduced some years ago in connection with spin glasses.[1] These are defined by a nearest-neighbor Hamiltonian

$$\frac{H}{kT} = -\sum_{\langle ij\rangle} J_{ij}\cos(\theta_i-\theta_j)\,, \tag{1}$$

where $J_{ij}=\pm J$ satisfy the "odd rule" in which the number of bonds with negative J_{ij} in an elementary plaquette is odd. For the triangular lattice, this constraint can be satisfied by isotropic antiferromagnetic couplings, while for the square lattice it can be satisfied by ferromagnetic horizontal rows and alternating ferromagnetic and antiferromagnetic columns. The Ising version of these models has no finite-temperature phase transition, but the *XY* version has a ground state with continuous U(1) and discrete Z_2 symmetry and has a phase transition of an unknown nature.

Most of the recent studies[2–17] of the phase transitions in this system have been mainly motivated by its relevance to Josephson-junctions arrays in a magnetic field. In fact, the model in Eq. (1) is a particular case of a more general class of uniformly frustrated *XY* models defined by

$$H/kT = -J\sum_{\langle ij\rangle}\cos(\theta_i-\theta_j-A_{ij})\,,$$

where the directed sum around an elementary plaquette $\sum A_{ij}=2\pi f$ and f is the uniform frustration. This is isomorphic to an ideal superconducting array if we identify $A_{ij}=(2\pi/\Phi_0)\int_i^j \mathbf{A}\cdot dl$, θ_i is the phase of the superconducting order parameter and Φ_0 the flux quantum. The vector potential $\mathbf{A}$ must satisfy $\nabla\times\mathbf{A}=\mathbf{B}$, the external perpendicular field, which identifies $f=\Phi/\Phi_0$ as the number of flux quanta per plaquette. The fully frustrated case corresponds to $f=\frac{1}{2}$.

In view of the continuous and discrete symmetry of the ground state of the *FFXY* model, one can introduce *XY* and Ising order parameters, and different scenarios are possible: Ising and *XY* transitions could occur at different temperatures giving rise to an intermediate phase; at the same temperature, but in a decoupled fashion, or, in the case of strongly coupled domain-wall and vortex excitations, a single transition in a different universality class could occur. There have been several numerical studies on the *FFXY* model on a triangular and square lattice, but no definite conclusions have been reached—even regarding the existence of an intermediate phase. Monte Carlo (MC) simulations yield apparently simultaneous occurrences of *XY* and Ising transitions on the triangular[4,12] and square[2,13,14] lattices, but a double transition with a *XY*-disordered and Ising-ordered intermediate phase has also been suggested.[3,15] The critical exponents associated with the Ising order parameter have been found to be consistent with the pure Ising values, even when a single transition is claimed. This view is usually supported by the observation that the finite-size dependence of the specific-heat maximum is consistent with a logarithmic behavior within errors. Generalized versions of the *FFXY* models have also been investigated. In some cases, Ising and *XY* transitions occurring at different temperatures can be identified when an appropriate parameter is changed.[13] However, the question of the double or single nature of the transition in the original model of Eq. (1) still remains.

Recently, the phase diagram of a coupled *XY*-Ising model of the form ($\sigma=\pm 1$)

$$\frac{H}{kT} = -\sum_{\langle ij\rangle}[A(1+\sigma_i\sigma_j)\cos(\theta_i-\theta_j)+C\sigma_i\sigma_j] \tag{2}$$

has been studied which is expected to describe the critical behavior of the *FFXY* model.[10,18,19] Early studies[6–9] of the model (2) have only considered the $C=0$ case. The triangular and square cases can be considered to lie along different paths in the parameter space (A,C). Depending on the parameters, separate *XY*, Ising, and first-order transitions were found. A line of continuous transitions was found with a simultaneous loss of *XY* and Ising order, and varying critical exponents. In addition, these exponents are found to be significantly different from the pure Ising values. The parameters of the square and triangular cases should lie close to the point where this single line bifurcates into two branches, one corresponding to pure *XY* transitions at low temperatures and another to pure Ising transitions at higher temperatures. These results then imply that in order to verify the single nature of the transition in the *FFXY* model, it is sufficient to study the Ising variables. If the critical exponents are inconsistent with the pure Ising values, the transition cannot be a decoupled Ising-*XY* or the Ising branch of a double transition. This point of view has the advantage of not requiring the very difficult determination of the helicity modulus jump which, in a model of this nature, does not have an obvious interpretation.

In this work we describe the results of a calculation of the critical exponents associated with the chiral (Ising) order parameter from a finite-size-scaling analysis of MC data. Using the same methods[20] applied to the coupled XY-Ising model,[19] we obtain $\nu=0.83(4)$ and $0.85(3)$, $2\beta/\nu=0.28(4)$, and $0.31(3)$ for the triangular and square lattices, respectively. These differ significantly from pure Ising exponents, and thus favor a single-transition scenario.

The MC simulations were carried out using a standard Metropolis algorithm in system sizes $6 \le L \le 40$ and periodic boundary conditions with small system sizes to perform long runs and achieve good statistics. Typically 5×10^6 MC steps were used in the simulations. The chirality order parameter[3,5] is defined as a directed sum around each elementary plaquette p as $\chi_p=(1/\gamma_0)\sum J_{ij} \times\sin(\theta_i-\theta_j)$ where the normalization factor $\gamma_0=3J\sqrt{3}/2$ and $2J\sqrt{2}$ for the triangular and square lattice, respectively. At zero temperature, $\chi_p=\pm1$, analogous to an antiferromagnetic Ising spin, and it is sufficient to consider the chirality per site χ of one of the sublattices.

From simulations at one temperature, we use the histogram method[21] to obtain information at nearby temperatures. If $-A_\chi(L,J)$ is defined as the logarithm of the histogram of chirality, the real bulk free-energy barrier $\Delta F_\chi(L,J)$ between ordered phases can be obtained from the depth of the minimum of A_χ as a function of χ.[20] At the transition, $\Delta F_\chi(\infty,J_c)=O(1)$, while for $T<T_c$, $\Delta F_\chi(L)$ increases with L as $L^{1/\nu}$ for $L \ll \xi$ (correlation length) and for $T>T_c$ approaches zero. This behavior near T_c is illustrated in Fig. 1. The change of behavior of ΔF_χ near T_c can be used to determine the critical temperature with good precision, and we find $T_c=0.513(2)$ and $T_c=0.455(2)$ for the triangular and square lattice, respectively. However, the exponent itself can be obtained quite easily from the slope of a log-log plot of $S=\partial\Delta F_\chi/\partial J \sim L^{1/\nu}$ as a function of L which yields $1/\nu$ from a one-parameter fit without requiring a precise determination of T_c, as in previous simulations. The exponent $2\beta/\nu$ can be obtained from the scaling of the location of the minimum in A_χ, which should scale as $L^{-\beta/\nu}$ at the critical point. This will depend on a precise location of the critical point, and hence is subject to larger uncertainty. In Fig. 2 we show a log-log plot of these quantities for the square and triangular lattices. A small curvature is still observed even for the largest system sizes, indicating that corrections to scaling are still important. However, considering system sizes with $L>10$, we obtain $\nu=0.83(4)$, $2\beta/\nu=0.28(4)$ (triangular), and $\nu=0.85(3)$, $2\beta/\nu=0.31(3)$ (square). These results differ significantly from the pure Ising exponents and seem to be consistent with the values obtained near the bifurcation point of a coupled XY-Ising model along the line of single transitions.[18,19] These values should be considered as upper bounds to the asymptotic result, since one can still detect a curvature in the data.

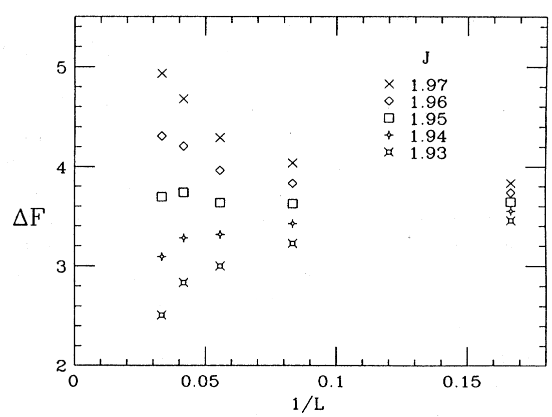

FIG. 1. Finite-size scaling of the free-energy barrier ΔF_χ for the triangular lattice.

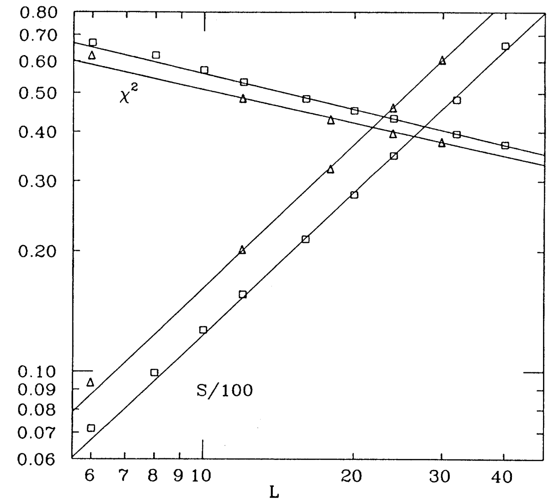

FIG. 2. Finite-size scaling of the minimum position χ^2 and $S=\partial\Delta F_\chi/\partial J$ for the square and triangular $FFXY$ models. The symbols correspond to square and triangular cases.

We have also made an independent estimate of the same critical exponents using the MC renormalization-group method.[22] Using the isolated block version of this method, we could use the same histograms. The effective exponents are obtained by comparing at T_c system sizes L and $L'=bL$ as $2\beta/\nu=\ln(\langle\chi_{L'}^2\rangle/\langle\chi_L^2\rangle)/\ln b$ and $1/\nu=\ln(\partial U_{L'}/\partial U_L)/\ln b$ with $U_L=1-\langle\chi_L^4\rangle/3\langle\chi_L^2\rangle^2$. In Fig. 3 we show the effective exponents for the triangular lattice obtained by this procedure. The estimate obtained by the previous method is indicated by arrows. Even though the extrapolation $\ln b \to \infty$ is not well defined, the trend of the data is in fair agreement with the estimate based on the scaling of ΔF_χ.

Recently, the exponents for the square $FFXY$ model have been evaluated[17] using a MC transfer matrix and the estimate of $2\beta/\nu$ agrees with our result within numerical uncertainties, but not for ν. We note, however, that ν was determined in an indirect way with several fitting parameters.[17] Our evaluation involves a one-parameter fit to the data and the result is definitely inconsistent with $\nu=1$.

Most of the evidence in favor of pure Ising exponents

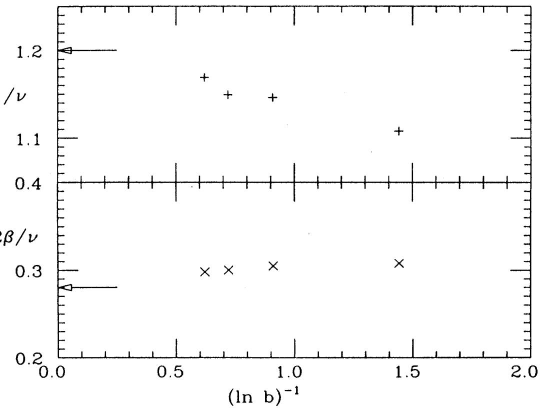

FIG. 3. Estimates of the exponents from the MC renormalization-group method for the triangular lattice. $L=6$ and $L'=bL$. Arrows indicate the results obtained from finite-size scaling of ΔF_χ.

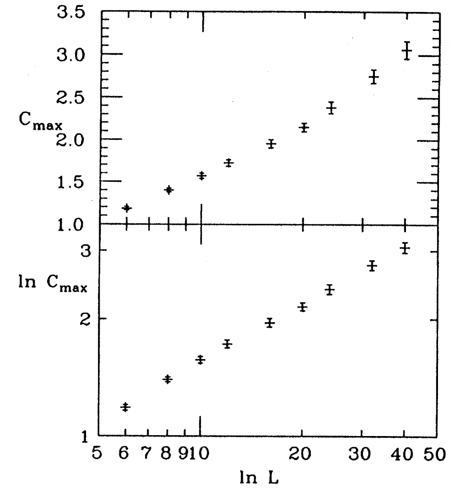

FIG. 4. Specific-heat maximum as a function of system size for *FFXY* model on the square lattice in a log-linear and log-log plot.

for the *FFXY* models relies on the finite-size behavior of the specific-heat maximum, which is usually found to be consistent with a logarithmic dependence on the size of the system, implying $\alpha=0$. However, it may be very difficult to distinguish a power law from a logarithmic divergence. To illustrate this point, in Fig. 4 we show the specific-heat maximum for the square lattice obtained from the data of ΔF_χ and compare the results of a log-log and log-linear plot. We note that the data is in agreement with the simulations of Ref. 2, in which a logarithmic behavior was suggested, but it is clear that at least for $L>10$ a better fit is obtained with a power-law divergence, from which we obtain $\alpha/\nu=0.48(7)$, from the largest system sizes. Using hyperscaling, this result is consistent with our estimate of ν from the finite-size scaling of ΔF_χ. For the triangular lattice, similar results are obtained with data in agreement with Ref. 3.

In conclusion, we have estimated the critical exponents of the *FFXY* models on a triangular and square lattice and found, contrary to previous simulations, that the chirality critical exponents are inconsistent with the pure Ising values. We argue that this result favors a single-transition scenario. Although the exponents agree within the estimated uncertainties, suggesting that the square and triangular cases may belong to the same universality class, simulations in larger systems sizes and better statistics may well result in different exponents. This nonuniversal behavior would be in complete agreement with the prediction, based on the results for coupled *XY*-Ising models.[18,19] Our approach allows us to obtain a very precise estimate of the temperature exponent $1/\nu$, independent of the exact critical temperature. We believe this method to be much superior to earlier ones because they rely on independent estimates of the Ising and *XY* transitions. The latter is extremely difficult to obtain in a model with an unknown critical behavior. The major impediment to large systems and good statistics is our use of the standard single-flip Metropolis algorithm. A modification allowing flipping of large blocks would improve the accuracy greatly and should allow us to reach asymptopia, and perhaps distinguish between exponents for the square and triangular lattices.

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