Critical behavior of the two-dimensional fully frustrated XY model

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We study the critical behavior of the fully frustrated XY model on a square lattice by means of extensive histogram Monte Carlo simulations. We find a single transition in contrast to the scenario of two distinct transitions. From a finite-size scaling we determine the critical exponents associated with the Ising-like order parameter and find $T_c(\infty)=0.4552(2)$, $\nu=0.852(2)$, and $\gamma=1.531(3)$. These exponents, different from the pure two-dimensional Ising critical exponents, are in agreement with the ones obtained for a mixed XY Ising system. [S0163-1829(98)00834-0]

I. INTRODUCTION

The critical behavior of two-dimensional (2D) fully frustrated (FF) XY model[1–3] has been the subject of many recent studies and controversies.[4–10] The reason for this increasing interest is that, despite of more than ten years of almost continuous investigations, the nature of the phase transition of this model is still not yet understood. Apart from a fundamental interest in the theory of phase transition in statistical mechanics where different approaches have been tested with this simple model, there is also an experimental interest since this system corresponds to a planar array of Josephson junctions in an external transverse magnetic field with the magnetic flux per plaquette given by half a flux quantum.[1] In this model there exits a discrete Z_2 symmetry of the Ising model in addition to the continuous U(1) symmetry associated to the global rotation of XY spins. The breaking of the former gives rise to an Ising-like transition while that of the latter to the Kosterlitz-Thouless (KT) one. There are several contradictory suggestions for these transitions: some authors say that the Ising and KT transitions occur at different temperatures, while others conclude that they take place at the same temperature.

On the one hand, in a generalized uniformly frustrated XY model where the frustration is varied by changing the negative bond strength[2,3] it has been concluded that the two transitions merge into a single transition in the fully frustrated case. This scenario of a single transition has been supported by a number of studies that give the following values for the critical exponent ν: $\nu=0.889$, (Ref. 7) and 0.813 (Ref. 6). These values are close to that obtained for the single transition in a mixed XY Ising model that is 0.85.[10,8] This suggests a new universality called XY Ising class for the transition occurring in this model. Very recently, Benakli and Granato[11] have introduced a generalized version of the square-lattice frustrated XY model where unequal ferromagnetic (F) and antiferrmagnetic (AF) couplings are arranged in zigzag pattern (see Fig. 1). They used a Ginzburg-Landau mean-field approximation and a finite-size scaling of standard Monte Carlo (MC) simulation to study the phase diagram and the critical behavior and showed that the transition is of the universality class of the XY Ising model. We note in passing that the question of new universality class arises also in the case of frustrated Heisenberg or XY spins on the stacked triangular antiferromagnet.[12]

On the other hand, other authors suggested two distinct phase transitions. Lee and Lee[6] have investigated the FF XY model on the square lattice using a microcanonical MC technique; they found two separate transitions, the KT transition at $T_{KT}=0.44$ and the Ising transition at $T_I=0.454$. Also, in the same model, by using the position-space renormalization group approach Jeon *et al.*[5] have showed that the KT-type transition and the Ising-like one occur at different temperatures. Olsson[4] has also found in the same model two distinct transitions. He calculated the chiral correlation function and then its coherence length from which he obtained $\nu=1$ as in the standard two-dimensional (2D) Ising model, in contradiction with results from previous papers cited above.

Given the contradiction between different approaches and MC results, we feel that it would be necessary to use a high-precision MC technique to study again this problem and to give definite answers to at least a few questions. The purpose of this paper is thus to use the so-called MC histogram technique[13] to study the phase transition of the FF XY model with zigzag couplings introduced by Benakli and Granato. The results shown below bring two definite conclusions: (i) they indicate a single transition and (ii) the values of the critical exponents are $\nu=0.852(2)$ and $\gamma=1.531(3)$, better than most earlier MC results, in agreement with the suggestion of a ''XY Ising universality class'' by Lee *et al.*[10,8,9]

In Sec. II we show the model and our results. Concluding remarks are given in Sec. III.

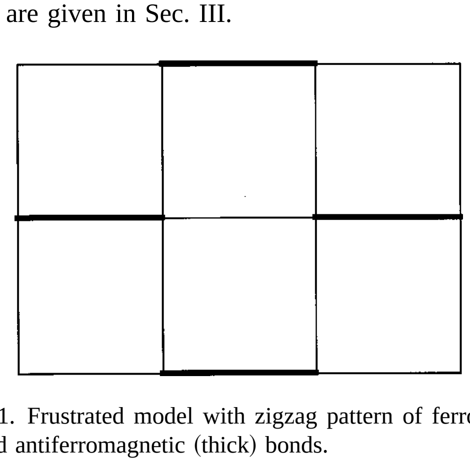
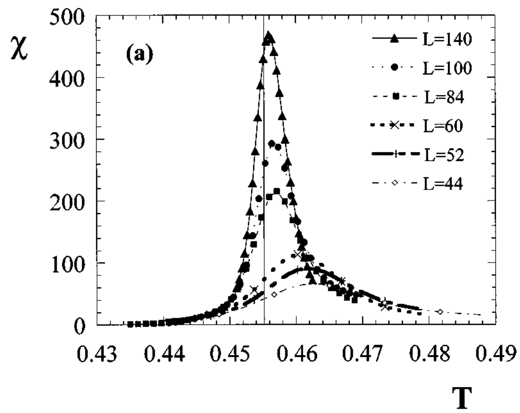


FIG. 1. Frustrated model with zigzag pattern of ferromagnetic (thin) and antiferromagnetic (thick) bonds.



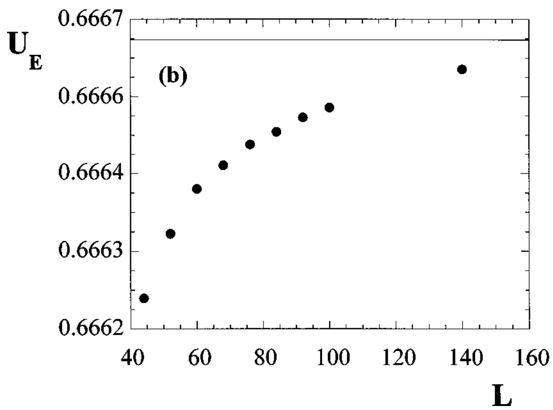


FIG. 2. (a) The chiral susceptibility χ [see Eq. (3)] as a function of T for different linear lattice size at $T_c(\infty)=0.4552(2)$. (b) The fourth-order energy cumulant [see Eq. (5)] vs L calculated at $T_c(\infty)=0.4552$. See text for comments.

II. MONTE CARLO HISTOGRAM SIMULATIONS

We consider the XY model on the square lattice where F and AF couplings are arranged in a zigzag pattern.[11] Our Hamiltonian is given by

$$H=-\sum_{(pq)} J_{pq}\mathbf{S}_p\cdot\mathbf{S}_q, \tag{1}$$

where $\mathbf{S}_p$ is an XY spin of unit length occupying the pth lattice site and the sum runs over nearest-neighbor (nn) pairs with exchange interaction $J_{pq}=J>0$ for F bonds or $-J$ for AF bonds. The classical ground state (GS) can be determined by the standard method, i.e., by minimizing the Hamiltonian.[2] The angle between two neighboring spins p and q is $\pm\pi/4$ for the F bonds and $\pm 3\pi/4$ for AF bonds. The GS energy is $E_0=-NJ\sqrt{2}$, where N is the total number of spins. J will be taken as a unit of energy hereafter.

We use in this work the histogram MC technique that has been developed by Ferrenberg and Swendsen.[13] We have used the system of $N=L^2$ spins where $L=44$ to 140 with periodic boundary conditions. We first estimate by standard MC simulation the transition temperature $T_0(L)$ as precise as possible for each lattice size L and then calculate the energy histogram $P(E)$ (E is the system energy) at that temperature. For the histogram calculation, we discarded $(1-2)\times10^6$ MC steps per spin for equilibrating the system and calculated the energy histogram as well as other physical quantities over the next 3×10^6 millions MC steps. Such long runs are necessary to get results of highest quality, as it is known in histogram technique. From $P(E)$ at $T_0(L)$, we calculate the following quantities at a temperature T close to $T_0(L)$:

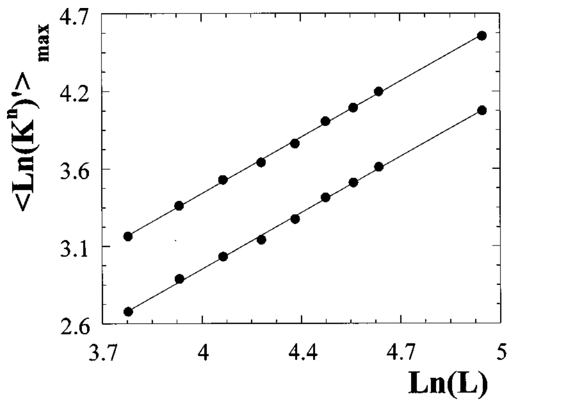


FIG. 3. $\langle(\ln K)'\rangle$ vs $\ln L$. The slope of the curve is equal to $1/\nu=1.173\,16$. $\langle(\ln K^2)'\rangle$ vs $\ln L$ (upper line) gives the same slope. The fitting error is less than 0.1%.

$$\langle C\rangle=\frac{(\langle E^2\rangle-\langle E\rangle^2)}{Nk_BT^2}, \tag{2}$$

$$\langle\chi\rangle=\frac{N(\langle K^2\rangle-\langle K\rangle^2)}{k_BT}, \tag{3}$$

$$\langle(\ln K^n)'\rangle=\frac{\langle K^nE\rangle}{\langle K^n\rangle}-\langle E\rangle, \tag{4}$$

$$U_E=1-\frac{\langle E^4\rangle}{3\langle E^2\rangle^2}, \tag{5}$$

$$U_K=1-\frac{\langle K^4\rangle}{3\langle K^2\rangle^2}, \tag{6}$$

where K is the chiral order parameter defined by

$$\mathbf{K}=\frac{1}{K_0N}\sum_m(-1)^m\sum_{\langle pq\rangle}(\mathbf{S_p}\wedge\mathbf{S_q})_m, \tag{7}$$

where K_0 being the value of K at $T=0$ is equal to $\pm\sqrt{2}/2$, m is the ordering number of plaquette, C the specific heat per site, χ the chiral susceptibility per site, U_K the fourth-order cumulant, U_E the fourth-order energy cumulant,[14] $\langle\cdots\rangle$ means the thermal average, and the prime denotes the derivative with respect to $\beta=1/(k_BT)$.

In all quantities, no evidence of two distinct phase transitions is found. Only one maximum is observed for each quantity. We show an example in Fig. 2(a) where the chiral susceptibility χ given by Eq. (3) is plotted as a function of T for $L=44$, 52, 68, 84, 100, and 140. Using the finite-size scaling for the maxima of $\langle C\rangle$, $\langle\chi\rangle$, $\langle(\ln K)'\rangle$, etc. we obtain the critical temperature for the infinite system which is $T_c(\infty)=0.4552(2)$. Note that the maximum of χ for the largest lattice size [Fig. 2(a)] is very close to the critical temperature $T_c(\infty)$ given above. The fourth-order energy cumulant U_E [see. Eq. (5)] has a minimum as a function of lattice size L at $T_c(\infty)$; in the thermodynamic limit the value

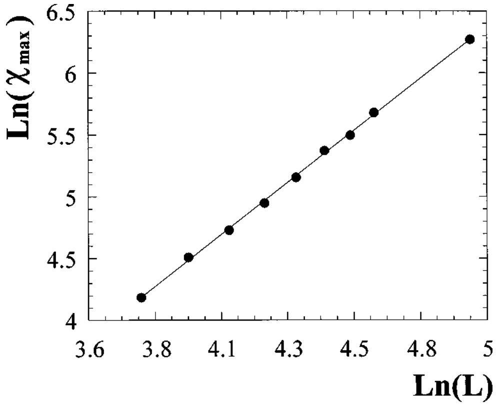


FIG. 4. Maximum of susceptibility χ as a function of L in a ln-ln scale. The slope yields $\gamma/\nu = 1.801\,15$ with fitting error less than 0.1%.

of this minimum tends to 2/3 for the continuous transition; this is presented in Fig. 2(b). The exponent ν can be obtained from the inverse of the slope of $\langle (\ln K)' \rangle_{max}$ and $\langle (\ln K)^2)' \rangle_{\max}$ versus $\ln L$. Our method for estimating the error is the following. (i) For each lattice size L, we estimate the transition temperature $T_0(L)$ as precisely as possible by standard Monte Carlo simulation. The error of $T_0(L)$ is $\pm\Delta$. Then we make histogram measurements at that temperature and calculate various physical quantities using Eqs. (2)–(6). (ii) Next, we make other histogram measurements at several temperatures (four to six) in the temperature region within the error of $T_0(L)$, i.e., from $T_0(L) - \Delta$ to $T_0(L) + \Delta$. For each histogram obtained, we calculate again various physical quantities. (iii) We average the calculated physical quantities and the resulting data point for size L is plotted in Fig. 3. Note that the error from this averaging is smaller than the size of the data point shown in these figures. (iv) We repeat steps (i) to (iii) for other lattice sizes.

The above method is known as multihistogram Monte Carlo technique. The results are shown in Fig. 3 where one observes an excellent straight line from which one obtains $\nu = 0.852(2)$. The fitting error is less than 0.1%.

This value is close to the one obtained by Lee and co-workers[10] using the coupled XY Ising model, but differs from $\nu = 0.813$ of Ref. 6 and from $\nu = 0.889$ of Ref. 7. The difference between our value of ν and these two values comes certainly from our very precise histogram technique.

The critical exponent γ is obtained by plotting $\ln\langle\chi\rangle_{\max}$ versus $\ln L$. We find $\gamma = 1.531(3)$ (see Fig. 4) where the error was estimated from the error of ν and the fitting procedure. This value of γ is also different from $\gamma = 1.448(24)$ given by Lee and Lee. The hyperscaling relations $d\nu = \gamma + 2\beta$ and $\alpha = 2 - d\nu$ give the $2\beta/\nu = 0.2$ and $\alpha/\nu = 0.35$, respectively. From these, one obtains $\beta = 0.08(2)$ and $\alpha = 0.30(1)$. Note, however, that these values are not obtained by direct calculations as for ν and γ. Their validity depends on that of the hyperscaling relations used. The obtained value of $2\beta/\nu$ is consistent with the previous results[6,7] but differs from the value $2\beta/\nu = 0.31(3)$ obtained by Lee and co-workers.[10]

III. CONCLUDING REMARKS

In summary, we have studied the phase transition of the fully frustrated XY model with zigzag couplings by extensive MC histogram technique. We find no evidence of two distinct phase transitions claimed by some authors.[6,5,4] On the contrary, all calculated quantities show clearly a single transition. We obtain in this work very precise values for the chiral critical exponents. These values are in agreement with but better than those of other recent MC simulations. They differ clearly from the pure Ising values (2D). Our result for ν is consistent with that found for the coupled XY Ising model,[10] though the values of other exponents are slightly different from those obtained by Lee and co-workers.[10] In spite of this difference that may be due to their MC procedure, we believe that the model studied here belongs to this coupled XY Ising model.

We think that this work brings two definite answers to the problem: the existence of a single transition and the precise values of the critical exponents ν and γ.

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