Finite size scaling and first-order phase transition in a modified *XY* model

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Monte Carlo simulation has been performed in a two-dimensional modified *XY*-model first proposed by Domany *et al.* [Phys. Rev. Lett. **52**, 1535 (1984)] The cluster algorithm of Wolff has been used and multiple histogram reweighting is performed. The first-order scaling behavior of the quantities such as specific heat and free-energy barrier are found to be obeyed accurately. While the lowest-order correlation function was found to decay to zero at long distance just above the transition, the next-higher-order correlation function shows a nonzero plateau.

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More than two decades ago Domany *et al.* [1] proposed a generalization of the two-dimensional *XY* model where the shape of the usual cos θ type potential could be modified with the help of a single parameter. The two-dimensional spins located at the sites of a square-lattice interact with the nearest neighbors through a potential

$$V(\theta_{ij}) = 2\left[1 - \left(\cos^2\frac{\theta_{ij}}{2}\right)^{p^2}\right], \tag{1}$$

where θ_{ij} is the angle between the spins and p^2 is a parameter used to alter the shape of the potential. For $p^2=1$ the potential reproduces the conventional *XY* model while for larger values of p^2 the potential well becomes narrower. The conventional two-dimensional *XY* model does not possess any true long-range order which is ruled out by the Mermin Wagner theorem. However a continuous quasi-long-range order-disorder transition resulting from the unbinding of topological defects [2,3] is known to occur in this system and the order-parameter correlation function is characterized by a slow algebraic decay instead of the fast exponential decay observed in a disordered system and this is referred to as the Kosterlitz-Thouless (KT) transition in literature. Domany *et al.* [1] performed Monte Carlo (MC) simulation and observed that as the potential well gets narrower with the increase in the parameter p^2, the continuous transition gets converted into a first-order phase transition and for $p^2=50$ the transition is very sharp as is manifested by a huge peak in the specific heat. This phenomenon is in apparent contradiction with the prediction of the renormalization group (RG) theory according to which systems in the same universal class (having same symmetry of the order parameter and same lattice dimensionality) should exhibit the same type of phase transition with identical values of critical exponents.

The generalized *XY* model of Eq. (1) has been analyzed by a number of authors [4,5] using the renormalization approach of the Migdal-Kadanoff type. These investigators were of the opinion that the transition in the generalized *XY* model appears to be first-order in nature because the MC simulation of Domany *et al.* [1] and Himbergen [6] were carried out on relatively small lattices and for large system sizes the usual KT transition is expected to occur. Nearly a decade later, Mila [7] using the same sort of renormalization group analysis arrived at a similar conclusion. Lastly, using the same line of approach, Garel *et al.* [8] put forward a different type of interpretation of the above-mentioned RG analysis and was of the view that the transition is indeed first order.

Minnhagen [9–11] has carried out a detailed study of the behavior of the phase transition exhibited by a two-dimensional (2D) Coulomb gas, which very well describes the characteristics of a 2D system consisting of vortex-antivortex pairs. It was demonstrated that the KT behavior is obtainable in a 2D Coulomb gas only at low particle densities. For higher particle densities the charge unbinding transition was shown to be first-order. Also a gas-liquid like critical point was found in the 2D Coulomb gas—the first-order line in the temperature-particle density plane ends at a critical point. The KT transition line, obtainable at lower densities was seen to join smoothly with the first-order line at a temperature slightly lower than the critical point. Jonsson *et al.* [12] performed MC simulation in a 2D *XY*-model with a modified potential, which essentially is equivalent to that of Eq. (1) and established a critical point. They determined the critical exponents for the system and interpreted the transition to be of the vortex unbinding type.

van Enter and Shlosman [13] presented a rigorous proof that various SO(n)- invariant n-vector models which have a deep and narrow potential well, would exhibit a first-order transition. The model represented by Eq. (1) is a member of this general class of systems. These authors based their proof on the so called method of reflection positivity, a technique borrowed from the field theory and used in statistical mechanics. van Enter and Shlosman argued that in spite of the order parameter in 2D n-vector model being predicted to vanish by the Mermin-Wagner theorem, long-range order prevails in the system via higher-order correlation functions. More recently, S. Ota and S. B. Ota [14] have performed MC simulation of the modified *XY* model using microcanonical ensemble and have identified a first-order phase transition in the system.

The present article describes MC simulation of the 2D modified *XY* model where computations have been performed on systems of reasonably large size and finite size scaling rules for first-order phase transition have been tested

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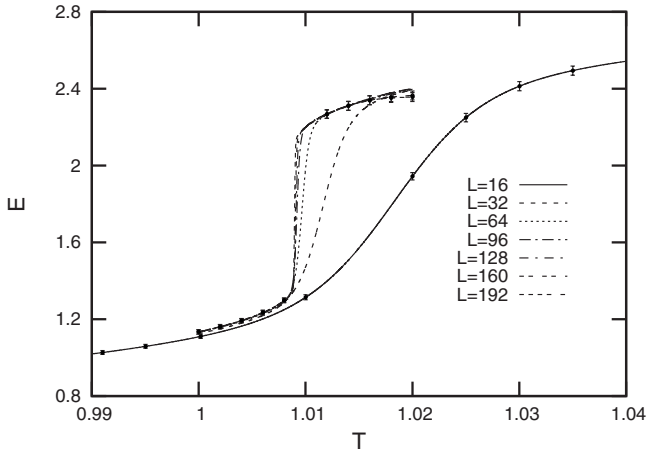

FIG. 1. The average energy per particle E plotted against dimensionless temperature T for different lattice sizes. For clarity error bars are shown only for $L=16$, 160, and 192.

on the results of the simulation. The motivation is to resolve the question on the nature of the phase transition in this model and the contradictions among the views put forward by different investigators for the last quarter of a century as has been summed up above. Our observation is that the transition is indeed first-order for a large value of the parameter p^2 (we have used $p^2=50$) as all finite size scaling rules are nicely obeyed. We however have made no attempt to investigate the existence of the critical point in this model or to determine the critical exponents as has been done by Jonsson *et al.* [12] in relatively small systems. Among other observables we have computed the spin-spin angular correlation functions of different orders. We observe that while the lowest-order correlation function decays to zero, the next-higher-order correlation function has a finite plateau which is in accordance with statement of van Enter and Sholsman [13].

Another interesting aspect of our work is the application of the Wolff cluster algorithm [15] to simulate the model. It has been pointed out by a numbers of workers [1,16] that the two-dimensional model is difficult to simulate using the conventional single spin-flip Metropolis algorithm [17]. To increase the reliability of the results we have used the multiple histogram reweighting, due to Ferrenberg and Swendsen [18] along with the Lee and Kosterlitz's method [19] of finite size scaling for a first-order phase transition. We observe that a combination of these computational tools until now provides a very efficient and accurate method of analyzing results obtained in an unknown system.

Square lattices of linear dimension L ranging from 16 to 192 were simulated and for each lattice simulations were performed at 9 to 13 temperatures in the neighborhood of the transition to record the histograms for energy. The number of configurations generated ranges from about 10^8 to 10^9. This was estimated from the values of the autocorrelation time for energy which we determined for all system sizes for each temperature. Figure 1 shows the temperature variation in the energy for a number of lattices, as is obtained by applying histogram reweighting technique. From the energy histograms, we have calculated the free energy like quantity A, defined as $A(E;\beta,L,\mathcal{N})=-\ln N(E;\beta,L)$, where $N(E;\beta,L)$ is the histogram count of the energy distribution. The free-energy barrier $\Delta F(L)$ was evaluated and in Fig. 2 we have plotted ΔF against L where a good linear fit has been obtained. This is a direct verification of the scaling rule $\Delta F \sim L^{d-1}$ of Lee and Kosterlitz [19] for a first-order phase transition since the lattice dimensionality $d=2$ in this model. We further note that the scaling relation is well obeyed down to $L=16$ which happens to be of the order of the correlation length, ξ for the system, as one can estimate from the relation $\Delta F(\xi) \simeq 1$ [19].

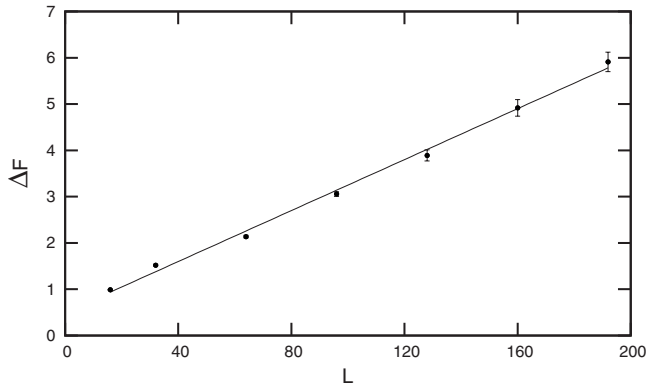

FIG. 2. The free-energy barrier height ΔF plotted against lattice size L with the linear fit represented by straight line.

The specific heat C_v was obtained from the energy fluctuation and Fig. 3 shows its temperature variation. It is evident that the peak height of C_v grows rapidly at the transition. From Fig. 4, where the maxima of C_v are plotted it is clear that the standard scaling rules $C_v \sim L^d$ for first-order transition [20] are accurately obeyed in this model.

We have also tested the finite size scaling relation

$$T_c(L) - T_c(\infty) \sim L^{-d}, \tag{2}$$

which is valid for a first-order phase transition [20]. $T_c(\infty)$ represents the thermodynamic limit of the transition temperature T_c. We have estimated the transition temperature in two

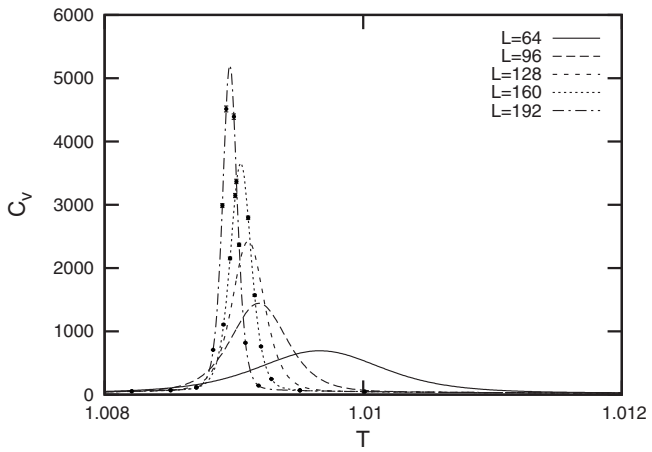

FIG. 3. The specific-heat C_v plotted against temperature T for different lattice sizes. For clarity only the above lattice sizes are shown and the error bars have been indicated for two lattice size.

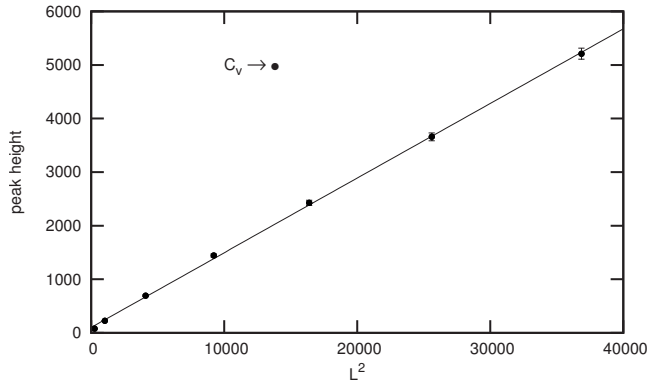

FIG. 4. The peak heights of C_v plotted against L^2 with the linear fit represented by the straight line. The error bars for most points are smaller than the dimensions of the symbols used for plotting.

ways—$T_c^{C_v}$ is the estimate of T_c obtained from the peak position of the specific heat C_v and T_c^F represents the transition temperature obtained from the fine tuning of the free energy vs energy curve to obtain two equally deep minima. In Fig. 5 the transition temperatures thus obtained have been plotted against L^{-2}. It is seen that the linear fits are good within statistical errors and the thermodynamic limit of the transition temperature is $1.008\ 97 \pm 6 \times 10^{-5}$, within which the two linear fits are seen to converge.

The first rank pair-correlation function is defined as

$$G_1(r) = \langle (\cos\ \theta_{ij}) \rangle_r, \tag{3}$$

where i and j are two spins separated by a distance r. The second rank pair correlation function is defined as

$$G_2(r) = \langle P_2(\cos\ \theta_{ij}) \rangle_r. \tag{4}$$

The pair-correlation functions $G_1(r)$ and $G_2(r)$ were calculated for temperatures $T=1.0081$, 1.0085, 1.0092, and 1.0095 for $L=128$ and are shown in Figs. 6 and 7. The first two of these temperatures are less than the transition temperature for this lattice while the other two temperatures are in the disordered phase. The curves have been fitted to a power law $G_i(r)=a_i r^{-b_i}+f_i$ for $i=1$ and 2. It may be noted that the parameter f is the asymptotic value of the pair-correlation function. We observe that while the first rank correlation function $G_1(r)$ decays to zero at the two higher temperatures ($f_1=0$), this is not the case for the higher rank correlation function $G_2(r)(f_2 \sim 0.22)$. In other words, while the lowest rank correlation among the spins vanishes just above transition, the next higher rank correlation continues to persist.

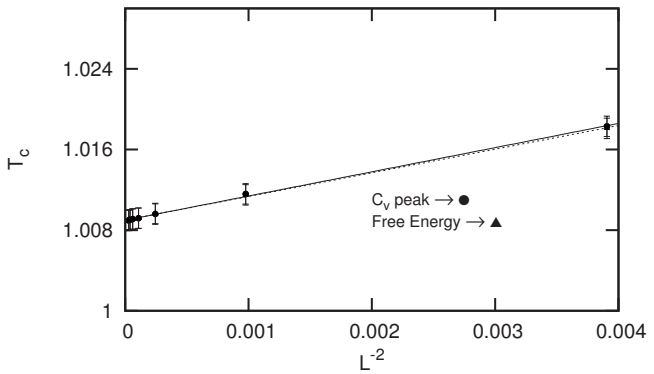

FIG. 5. The transition temperature T_c obtained from (a) specific-heat peak position and (b) fine tuning of free energy curve plotted against L^{-2} along with the respective linear fits. The intercept on the Y axis is $1.008\ 97 \pm 6 \times 10^{-5}$.

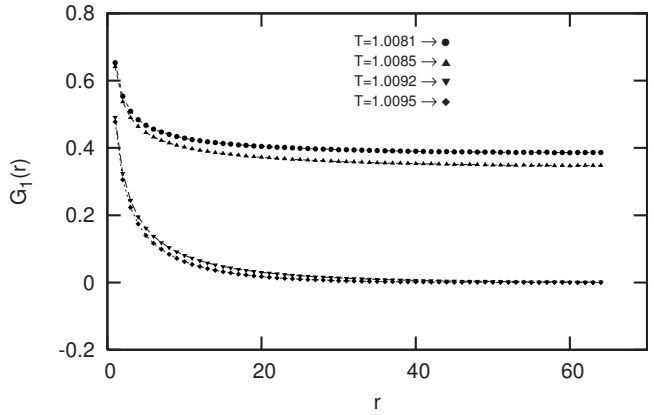

FIG. 6. The plots of the pair correlation function $G_1(r)$ against r for the 128×128 lattice for the temperatures indicated. The curves are plotted for r ranging up to $L/2$.

The simulations in the two-dimensional modified XY model presented in this communication show that all the first-order finite size scaling rules are obeyed. Computation has been performed in system size up to 192×192 which may be considered to be reasonably large for the purpose of arriving at a conclusion regarding the behavior of the model. We are inclined to conclude that the model exhibits a first-order phase transition. This is in agreement with the views of some of the earlier investigators including Domany *et al.* [1] and van Enter and Shlosman [13]. The existence of a quasi-long-range order-disorder transition observed in the 2D XY model is known to be due to vortex-antivortex unbinding (KT transition). In absence of the role played by the vortices, one would not observe any order-disorder transition in the XY model in accordance with the Mermin-Wagner theorem. In the class of models we have investigated the role played

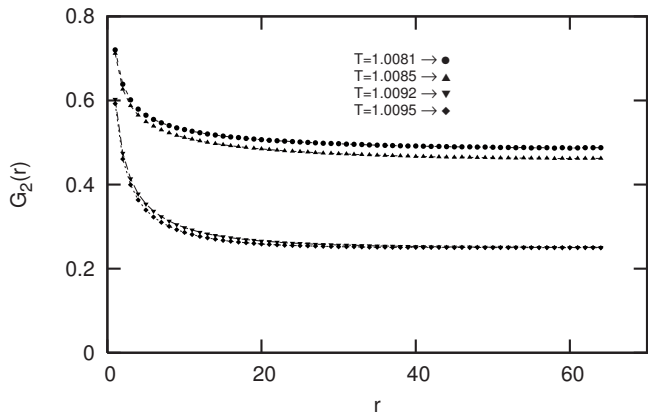

FIG. 7. The plots of the pair correlation function $G_2(r)$ against r for the 128×128 lattice for the temperatures indicated. The curves are plotted for r ranging up to $L/2$.

by the vortices changes qualitatively with change in p^2 (which increases the nonlinearity of the potential well) as has been seen in the early work of Himbergen [6]. Also we have seen that the number of vortex pairs grows rapidly with the increase in p^2 [21]. Qualitatively, one may therefore think that the modified XY model for large values of p^2, behaves like a dense defect system and gives rise to a first-order phase transition as has been predicted by Minnahagen [9–11].

We mention another point before ending this section. This is the performance of Wolff cluster algorithm which turned out to be very convenient to simulate the model. Conventional algorithms, as we have seen, do not work well in this model. Our earlier attempt [16] using the recently developed Wang-Landau (WL) algorithm [22] which directly determines the density of states of a system is also not a good choice for simulating this model. The main problem while using the WL algorithm is that configurations near the minimum energy take a very long time to be sampled during the random walk and it becomes impractical to simulate continuous models of even moderate size because of the huge CPU time that becomes necessary. Among other things, a great virtue of the Wolff algorithm is that it does not contain any adjustable parameter even while simulating a continuous model.

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