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Microcanonical Monte Carlo Simulations of First-Order Transition in a 2D XY-model

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Abstract:
We have studied the first-order transition in the two-dimensional classical XY-model with the modified nearest neighbour interaction potential suggested by Domany, Schick and Swendsen. Microcanonical Monte Carlo simulations have been carried out with 25, 100 and 900 spin systems on a square lattice with periodic boundary conditions. The first-order transition temperature is found to decrease with the increase in system size. The physical variables such as mean square magnetisation per spin and vorticity have been obtained in the transition region using this technique. It is found that the creation of a vortex-antivortex pair costs more energy during the transition than the energy associated with a bound pair.

Study of phase transition in classical XY-model in two dimensions has attracted remarkable degree of attention[1]. Some of the notable properties of this model are the absence of long-range order, the presence of topological defects called vortices and the Kosterlitz-Thouless (KT) transition[2-4]. The low temperature phase has only bound vortex-antivortex pairs and the KT transition is associated with the unbinding of vortex-antivortex pair. Investigations have been carried out on the possibility of a first order transition without disturbing the essential symmetry[5]. Recently, Domany, Schick and Swendsen[6] suggested a modification of the nearest neighbour interaction potential in this model. By appropriate choice of the parameter in this potential a first-order transition is observed. Several canonical Monte Carlo simulations have been carried out to study this spin model with continuous symmetry[7,8]. It is however, not practicable to study the behaviour in the transition region using canonical Monte-Carlo simulations[9], where temperature is the input parameter. This arises because the physical variables show step-like behaviour at the transition temperature in the case of a first-order transition. This aspect can however, be studied by the Monte Carlo simulation method proposed by Creutz[10]. It differs from the metropolis algorithm[9] in operating within a microcanonical ensemble, so that the energy is fixed (input parameter) and the temperature is obtained from the simulations, not vice versa. This provides an advantage because the physical quantities depend in a smoother way on the system energy than on the temperature, at the first order transition. Harris[11] has used this method of Creutz to study the first order transition in a discrete Ising-like spin-model.

Recently, we developed an algorithm to implement this technique for spin systems with continuous symmetry (the two dimensional (2D) classical XY-model)[12]. In this work, we report the study of the first order transition in a 2D classical XY-model with the nearest neighbour interaction potential suggested by Domany, Schick and Swendsen[6]. Using this algorithm, we clearly demonstrate its potential for the study of the transition region.

The Hamiltonian of the classical 2D XY-model, as suggested by Domany, Schick and Swendsen is given by:

$$H = 2J \sum_{<i,j>} [1 - (cos^{2p^2} \frac{\theta_i - \theta_j}{2})], J > 0, \quad (1)$$

where $J > 0$ is the coupling constant and θ_i is the angle made by the spin at site i with respect to a fixed axis in the plane. The sum $< i,j >$ is over the nearest neighbours. For $p^2 = 1$ the Hamiltonian reduces to the usual classical 2D XY-model. By increasing p^2 the potential well can be made narrower and for $p^2 > 10$ the transition becomes first-order in nature. Recent canonical Monte Carlo simulations also support the first-order nature of this transition[8].

For our simulation, we chose $p^2 = 50$ in Eq.1 and consider a 2D square lattice having 25, 100 and 900 spins with periodic boundary condition. For simplicity and faster computational speed, the continuous θ is descretised. We used 300 descrete states; $\theta_i = 2\pi n/300$, where n=1,2,3, ...,300. The microcanonical MC simulations were carried out as discussed in Ref.12.

Typically we used 4×10^4 Monte Carlo Step per Spin (MCSS) for equilibration and 6×10^4 MCSS for averaging. The averaging was carried out in 12 blocks with 5×10^3 MCSS per block for the estimation of standard deviation of the physical variables such as mean square magnetisation per spin and vorticity. The temperature dependence of the spin system energy (E_s) is displayed in Fig.1. (Here we have replaced k_BT/J by T and E/J by E.) The linear temperature dependence of E_s seen at low tempetatures is due to the spin wave behaviour.

The equilibrium mean square magnetisation per spin is calculated as follows:

$$N^{-1} < M^2 >= N^{-1} < (\sum_{i=1}^{N} cos\theta_i)^2 + (\sum_{i=1}^{N} sin\theta_i)^2 >, \qquad (2)$$

where N is the total number of spins. Fig.2 displays $N^{-1} < M^2 >$ as a function of temperature. Similarly, the vorticity in each elementary square plaquette (consisting of four spins at the corners), was also calculated[1]. The total number of positive vortices was found to be equal to the total number of negative vortices, which is a consequence of the periodic boundary conditions. Fig.3 displays the temperature dependence of vorticity.

It is seen that the temperature dependence of E_s, $N^{-1} < M^2 >$, and vorticity show a step-like change at 1.01, which corresponds to the first order transition temperature T_c. Simulations on 25 and 100 spin systems were carried out with 2×10^4 MCSS for equilibration and 3×10^4 MCSS for averaging (in 12 blocks with 2500 MCSS per block). Average over three

energy values was taken to obtain the transition temperature. We obtain T_c of 1.11 (1.04) for 25 spin (100 spin) system. We note that T_c increases with decrease in system size. From this behaviour, T_c of 1.00 is expected in the thermodynamic limit. This value of T_c is in good agreement with the result from canonical Monte Carlo simulations on systems of comparable size[6,7].

The physical picture for the origin of the first-order transition is as follows. For small p, the potential well of the nearest neighbour interaction is rather wide, so that vortices and antivortices enter the system gradually as the temperature is increased and at the Kosterlitz-Thouless transition temperature there is a dissociation of the bound vortex-antivortex pair. For large p, the potential well is narrow and there is an insufficient increase of vortex density at low temperature. Then at a fixed higher temperature there is a sudden appearance of large number of vortex-antivortex pairs, resulting in a first-order transition. This feature is clearly seen in Fig. 3. In the present simulation values of vorticity and magnetisation have been obtained also in the transition region, which were absent in the earlier canonical Monte Carlo simulations. We also observed that the values of vorticity for a fixed system energy, in the heating cycle is lower than the corresponding value in the cooling cycle. This difference is due to the metastability of the system in a first-order transition. From the energy dependence of vorticity, of the 900-spin system, we estimate that the creation of a vortex-antivortex pair costs about 19 units of energy in the transition region, compared to 14 units of energy for the closest bound pair. This implies that during the transition majority of the energy is spent in the creation of bound vortex-antivortex pair. It is important to note that, in an experimental study of the first order transition, energy is added to (removed from) the system and the resulting physical quantities are measured. During the transition, the temperature remains constant. The microcanonical Monte Carlo simulations closely represents this situation and therefore, is expected to give reliable results of the transition.

In conclusion, we have demonstrated the potential of the microcanonical Monte Carlo simulations in the study of first order transition. We have obtained vorticity and magnetisation in the transition region for the modified potential in case of 2D classical XY-model. It is observed that the creation of a vortex-antivortex pair costs about 19 units of energy in the transition region.

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Fig-1

Figure Captions:

Figure 1: Average system energy per spin as a function of temperature for 900 spin system.
Figure 2: The mean square magnetisation as a function of temperature for 900 spin system.
Figure 3: Vorticity as a function of temperature for 900 spin system.

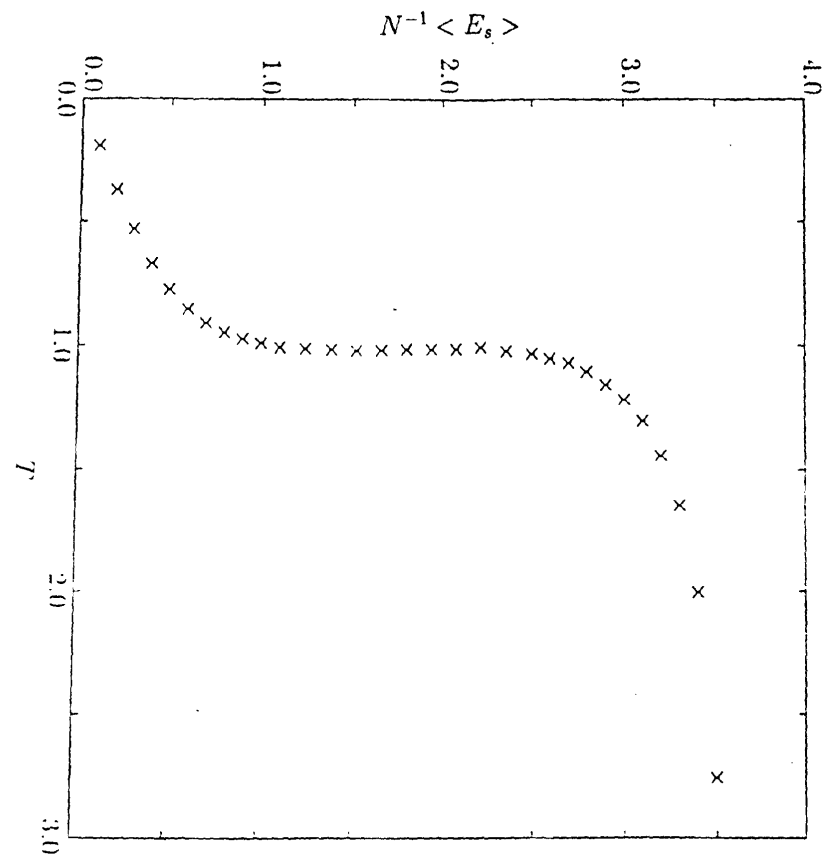

Fig-3

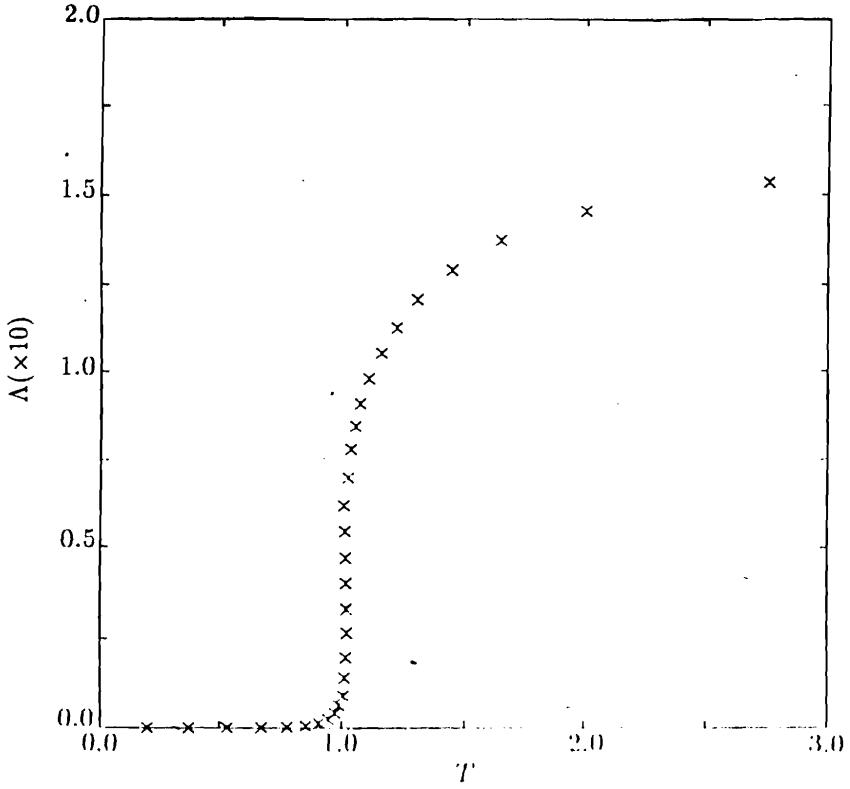
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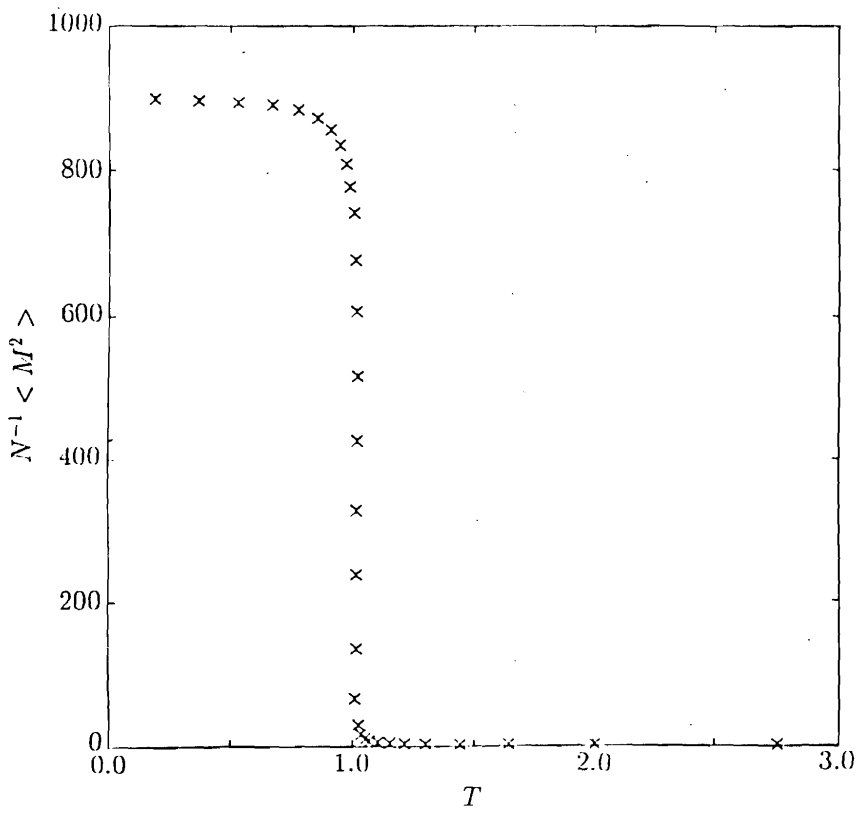
Fig-2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