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Nature of First-Order Transition in Planar Rotator Model with Modified Potential

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ABSTRACT

We have carried out micro-canonical Monte Carlo simulations of a planar rotator model in 30×30 lattice using periodic boundary conditions. The energy distribution of the rotator in the lattice shows features that can be associated with spin wave and vortex excitations. The results supplement the first-order transition observed in canonical Monte Carlo simulation, due to vortex nucleation. We also see features that can be associated with the in-homogeneity of vortex charge in the critical region.

Keywords: XY-Model; Spin Wave; Vortices

1. Introduction

Simulations of statistical systems have gained much interest, recently [1-4]. The spin-models with continuous symmetry, such as the planar rotator model [5], has been studied significantly to know its properties and applicability to physical systems. In the past, effort has been made to know the type of phase transition in a magnetic material through planar rotator model [6]. It has also been used to study exotic materials such as high temperature superconductors [7] and super-fluids [8]. It is known that the planar rotator model shows several important properties: such as lack of long range order, the presence of topological defects called vortices, the vortex unbinding transition called Kosterlitz-Thouless (KT) transition, which is topological in nature [9-14]. The behavior of the system is known to be accurately described at sufficiently low temperatures by the "spin-wave" theories by Wegner [12] and Berezinskii [13] and later by Zittartz [14]. Various theoretical techniques have been used to study the spin waves and vortices [14,15]. Several canonical Monte Carlo (MC) simulations [16-22] have been carried out using the Metropolis procedure [23]. There are also studies with canonical MC simulations based on improved techniques [24-26] and the micro-canonical molecular dynamics algorithm [27]. Being of a topological nature, no specific heat anomaly is observed at the KT transition temperature T_{KT}. But the temperature dependence of the specific heat shows a peak at a temperature, which is about 15% higher than T_{KT}.

It has been found that the vortex unbinding transition temperature (T_v) increases by reducing the potential well width. On the other hand, local disorder sets in at temperatures near the potential well height

$$T_D \approx V(\pi) - V(0) = 2J .$$

Therefore, for a sufficiently narrow potential well $T_D < T_v$, we expect the continuous transition to yield to a first-order vacancy condensation transition. Several studies have been carried out to understand the first order transition in this system [28-48]. Here we report the study of the nature of the first order transition in a finite isolated system, which supplements the results observed in canonical Monte Carlo simulations [28,29].

The Hamiltonian of the planar rotator model with modified potential is given by:

$$H = 2J \sum_{\langle i,j \rangle} \left\{ 1 - \cos^{2q} \left[\left(\theta_i - \theta_j \right) / 2 \right] \right\} \quad (1)$$

J in Equation 1 denotes the interaction strength (>0 for the ferromagnetic case) and the sum is over all the nearest neighbors [28]. In Equation (1), $q = p^2$ is the controlling parameter and $q > 0$. As q is raised, it has an increasingly narrow well of width $\approx \pi / \sqrt{q}$ and for $\theta > \pi / \sqrt{q}$ it is essentially constant at $V(\pi) = 2J$. For $q = 1$, the Hamiltonian gives rise to the Kosterlitz-Thouless transition and for large value of q, the transition is first-order in nature.

We performed micro-canonical Monte Carlo (MC) simulations [49,50] on 30×30 rotator system using the Hamiltonian given in Equation (1). There are also other

simulation methods which have been reported recently [51,52]. We used periodic boundary conditions. It is known from renormalization group theory that fluctuations at all wave lengths are equally important around the phase transition [53]. For a 30 × 30 system, the boundary to area ratio is nearly 8 and therefore, one expects to see features of a large system. In the simulations there is an extra degree of freedom which exchanges energy with the rotator system. The temperature is directly related to the average energy of the extra degree of freedom $\langle E_D \rangle$:

$$\langle E_D \rangle = k_B T \qquad (2)$$

where k_B is the Boltzmann constant. (Hereafter we replace $k_B T/J$ by T and E/J by E for simplicity). In these simulations the total energy (E) is an input parameter and the temperature (T) is determined from the simulations. The system was heated in steps across the first order transition during which energy was added to the rotator system through the demon. **Figure 1** shows the energy as a function of temperature for $q = 55$. We used 5×10^5 Monte Carlo step per rotator (MCSR) for equilibration and 5×10^6 MCSR for averaging. We performed block averages consisting of 5×10^4 MCSR each and then found the standard deviation of the block averages. The standard deviation of the estimated temperature is less than about 0.5 percent. It is seen that the temperature dependence of energy shows a van der Waals-like loop at the first order transition, which occurs at $T = 1.0$. It is well known that meta-stability gives rise to van der Waals-like loop [54]. For instance; it arises in weak-long-range-force models. In the limit of infinite interaction range, the free-energy required towards a change to the equilibrium state is extensive and the mean-field approximation predicts that meta-stability lifetimes are infinite in the thermodynamic limit. We expect that such situation does not arise in the present study of finite systems. We note here that the canonical and the micro-canonical ensembles are mathematically linked by the Laplace transform [55] and the micro-canonical results can be obtained from the canonical energy distribution $P_{\beta,L}(E)$ by the following equation [56]:

$$\beta_{micro,L}\left(E/V\right) = d/dE\left[\ln\left(P_{\beta,L}\left(E\right)\right)\right] + \beta \qquad (3)$$

We studied the system (was studied) for various energy values with 5×10^6 MCSR for equilibration and 5×10^6 MCSR for averaging. The standard deviation of the estimated temperature in this set, is also less than about 0.5 percent. We studied the energy distribution of a rotator in lattice after equilibration. **Figures 2-4** show the energy distribution of the rotator in the lattice for various values of total system energy. In **Figure 2** the values of E lies below that at the transition. It is seen that there is a broad peak after which the energy shows an exponential distribution.
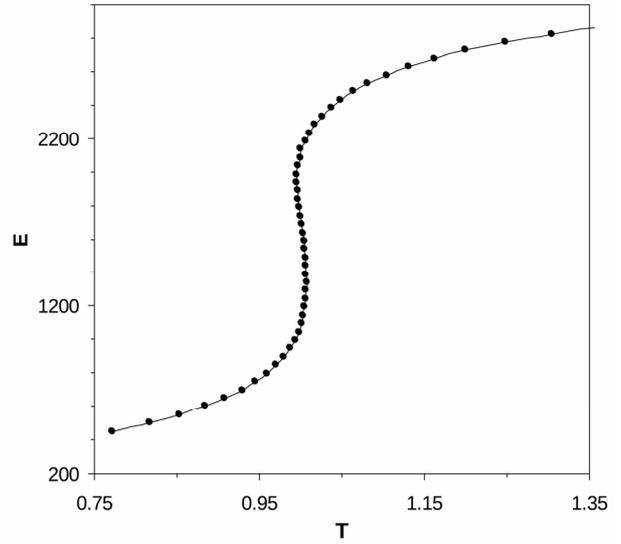

Figure 1. Temperature versus energy of the planar rotator model. The simulations are carried out on a 30 × 30 square lattice using periodic boundary conditions with $q = 55$. The van der Waals-like loop is observed at the first-order transition.
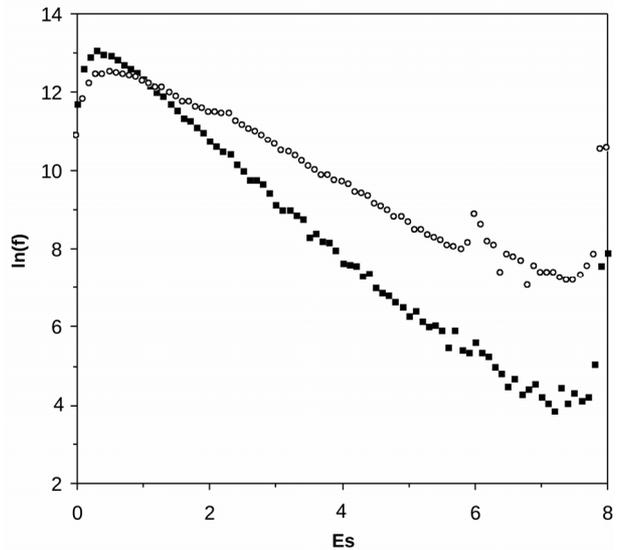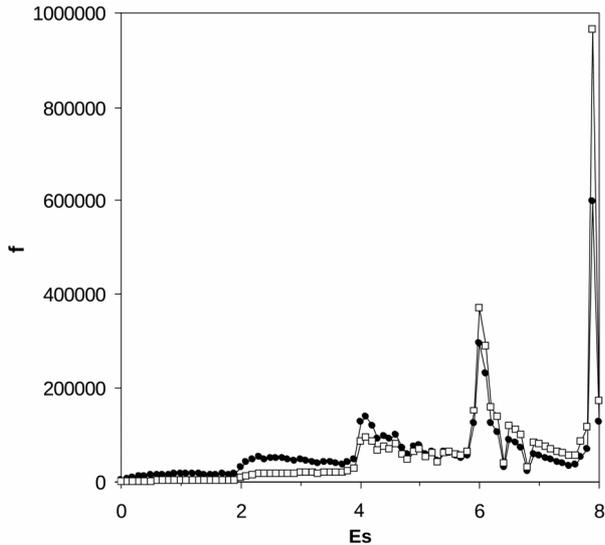

Figure 2. The frequency distribution of a rotator in the lattice for $E = 400$ ($T = 0.717$) (■) and $E = 700$ ($T = 0.930$) (○), which lie at low temperatures, below the first order transition: The ordinate represents the natural logarithm of the number of times out of the 5×10^6 MCSR that the rotator is in the corresponding energy bin of width 0.1.

We attribute this as due to the spin waves. In **Figure 3** the values of E corresponds to that at the transition. It is seen that a peak at $E_s = 7.9$ develops gradually apart from the broad low temperature peak which reduces in magnitude. There are also several intermediate peaks. In **Figure 4**, at high temperatures (above the transition), the broad low temperature peak is observed to be
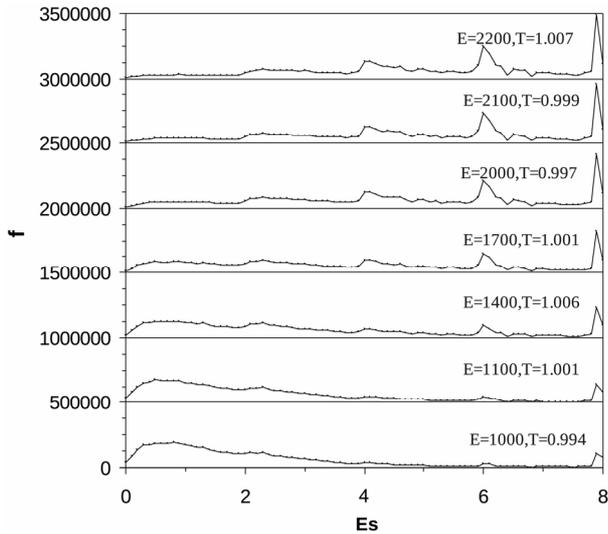
Figure 3. The frequency distribution of a rotator in the lattice for a range of system energies (temperatures) at the first order transition temperature: $E = 1000$ ($T = 0.994$) (lowest curve); 1100 (1.001); 1400 (1.006); 1700 (1.001); 2000 (0.997); 2100 (0.999); 2200 (1.007) (top most curve). The solid lines through the data are guide to the eye. The successive graphs are shifted along the ordinate by 5×10^5. The ordinate represents the number of times out of the 5×10^6 MCSR that the rotator is in the corresponding energy bin of width 0.1.


Figure 4. The frequency distribution of a rotator in the lattice for $E = 2400$ ($T = 1.041$) (●) and $E = 2800$ ($T = 1.273$) (□), which lie at high temperatures, above the first order transition. The ordinate represents the number of times out of the 5×10^6 MCSR that the rotator is in the corresponding energy bin of width 0.1. The solid lines through the data are guide to the eye.

absent and the peak at $E_s = 7.9$ continues to increase, along with the intermediate peaks. We attribute the high energy peak as due to the vortices. The height (or inten-

sity) of the peaks which arises due to spin waves and vortices is shown as a function of system energy in **Figure 5**. It is seen that the peak due to the spin waves reduces as the energy increases and at the end of the transition this peak is practically absent. However, on the other hand, the peak due to the vortex excitations continue to increase above the first order transition.

It is known that, the spin waves dominate at low temperatures [12-14]. The broad peak at low temperatures (**Figure 2**), can be attributed as due to such excitation. The peak at $E_s = 7.9$, is close to the value of energy needed to create a vortex-anti-vortex pair. The energy needed to create a vortex-anti-vortex pair (2μ) can be estimated from the expected exponential temperature dependence of vortex density: $V \sim e^{-2\mu/T}$ [18]. We obtain a value of $2\mu = 7.3$ [57]. The low temperature value of 2μ corresponds to the energy associated with the closest bound vortex-anti-vortex pair. This can be compared with the vortex-anti-vortex pair in the absence of a spin wave with lowest energy configuration [42]. The corresponding energy is 8 in units of J. Recently, the vortices in the classical planar rotator have been studied using canonical MC simulations based on an improved technique. The value of $2\mu = 7.55$ obtained in the simulations are in good agreement with the present results [25]. We note here that the analytical value estimated by Kosterlitz and Thouless is 9.9. Therefore, this peak at $E_s = 7.9$, can be attributed as due to vortices.

Simulations have shown that the vortex charge distribution is inhomogeneous [58]. The maximum in-homogeneity occurs at a temperature that corresponds to that of the coexistence region. Although we have not yet found an exact explanation of the observed in-homogeneity
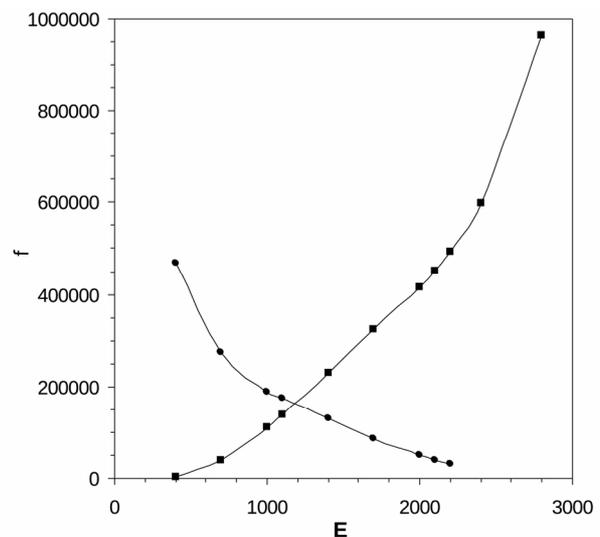
Figure 5. The intensities of the peak due to spin waves (●) and vortices (■) as a function of system energy. The solid lines through the data are guide to the eye.

of the vortices, certain features can be understood as follows. In the low temperature (energy) insulating phase the vortices are bound tightly which results in a small value of the vortex in-homogeneity. In the high temperature (energy) Debye-Hückel regime, the in-homogeneity is also small due to the presence of a large number of free charges in the liquid phase. We speculate that cluster of vortices in the critical region are responsible for the peak in the vortex charge in-homogeneity. The intermediate peaks seen in **Figures 3** and **4** can be attributed as due to the vortex-charge in-homogeneity.

In conclusion, we have studied the energy distribution of the rotator in the lattice. The energy distribution of the rotator, shows features that can be associated with spin wave and vortex excitations. The results substantiate the first-order transition observed in canonical Monte Carlo simulation, due to vortex nucleation. We also see features that can be associated with the in-homogeneity of vortex charge in the critical region.

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