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Micro-canonical Monte Carlo simulation of spin wave in 2D classical XY-model

Abstract

We have carried out micro-canonical Monte Carlo simulations of the two dimensional (2D) XY-model in a 30×30 lattice using periodic boundary conditions. The energy distribution of the spins in the lattice has been studied. The temperature dependence of the spin wave energy is determined from the average and the most probable energies of the spins; which is found to be in good agreement with that predicted from the spin wave theory. The vortex unbinding transition takes place, when the frequency of the most probable spin-wave energy reduces by one order of magnitude.

Key Words

XY-model; Spin waves; Vortices.

Statistical simulations have been powerful alternative to theoretical and experimental research.[1] It is known that the XY model shows several important properties[2-12]; such as lack of long range order, the presence of topological defects called vortices, the vortex unbinding transition called Berezinskii-Kosterlitz-Thouless (BKT) transition, which is topological in nature. The behavior of the system is known to be accurately described at sufficiently low temperatures by the 'spin-wave' theories. Various theoretical techniques have ben used to study the spin waves and vortices. Several canonical Monte Carlo (MC) simulations have been carried out. There are also studies with canonical MC simulations based on improved techniques and the micro-canonical molecular dynamics algorithms. 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}. Recently, the topological phase transition in 2D spin model with rotational symmetry (XY model) has been the focus of physics research[13]. The classical micro-canonical Monte Carlo simulations have quantum counterpart, which is useful for the study of finite quantum systems[14].

In this article, we describe how the spin wave and vortex excitations appear in the context of most probable energy of the spins in micro-canonical ensemble which has not been reported so far in the literature[15,16].

The Hamiltonian of the XY model is given by:

$$H=-J\Sigma_{<i,j>} \cos(\theta_i-\theta_j) \quad (1)$$

J in Eq.1 denotes the interaction strength (>0 for the ferromagnetic case) and the sum is over all the nearest neighbors. The Hamiltonian of the XY model with modified potential is given by[17]:

$$H=2J\Sigma_{<i,j>}\{1-\cos^{2q}[(\theta_i-\theta_j)/2]\} \quad (2)$$

In Eq.2, $q=p^2$ 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 Berezinskii-Kosterlitz-Thouless (BKT) transition and for large value of q, the transition is of first order in nature.

We performed micro-canonical Monte Carlo (MC) simulations on a 30×30 spin system using the Hamiltonian given in Eq.1[18-20]. There are also other simulation methods which have been reported recently. 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. For a 30×30 system, the boundary to area ratio is nearly 8 and therefore, one expects to see features of a large system. For simplicity and faster computational speed, the continuous θ is discretized. We used 300 discrete states; $\theta_i=2\pi n/300$, where n=1,2,3,...,300. Some specific features of this simulation program in FORTRAN is the use of intrinsic random number generator. We use the RAN function in the FORTRAN compiler with ISSED=425001 to generate the random numbers. The orientation of the spins is discretized and an integer 2D array is used to store the configuration of the spins. During the Monte Carlo updating, the involved energy is calculated using the integer configurations with a tabulated value of the corresponding energy of the spins. Finally, using this simulation it is easy to see the determination of thermodynamic quantities from a statistical simulation.

In the simulation there is an extra degree of freedom which exchanges energy with the spin system. The temperature is directly related to the average energy of the extra degree of freedom $<E_D>$:

$$<E_D>=k_BT \qquad (3)$$

where k_B is the Boltzmann constant. (Hereafter we replace k_BT/J by T and E/J by E for simplicity). In case of discrete spin model, such as the Potts model, the E_D takes energy values that are integral multiples of J. Therefore, one finds the following equation, valid for the Potts model, to determine the system temperature from the average demon energy:

$$kT=1/\ln(1+<E_D>^{-1}) \qquad (4)$$

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 spin system through the demon. We studied the system for various energy values with 5×10^6 Monte Carlo step per spin (MCSS) for equilibration and 5×10^6 MCSS for averaging. The standard deviation of the estimated temperature was less than about 0.5 percent.

We studied the energy distribution of a spin with its four nearest neighbors in the 30x30 lattice after equilibration. Figure 1 shows the energy distribution of the spin for q=1, in the lattice for various values of total system energy. It is seen that there is a broad peak, which shifts to higher energy as the temperature is increased. We attribute this as due to the spin wave excitations.

It is known that, the spin waves dominate at low temperatures. The broad peak at low temperatures (figure 1), can be attributed as due to the spin wave excitations.

The energy of spin waves can be shown to be given by:

$$E_{sw}=-2+\tfrac{1}{2}T \qquad (5)$$

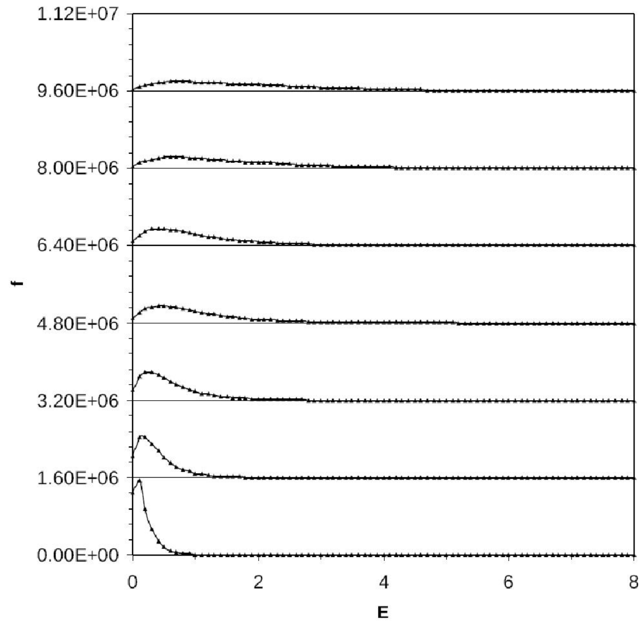

Figure 1 : The frequency distribution of a rotator in the lattice for a range of system energies (temperatures) with q=1: E=100 (T=0.216) (lowest curve); 200 (0.417); 300 (0.602); 500 (0.896); 600 (0.996); 736 (1.097); 836 (1.177) (top most curve). The solid lines through the data are guide to the eye. The successive graphs are shifted along the ordinate by 1.6×10^6. The ordinate represents the number of times out of the 5×10^6 MCSS that the rotator is in the corresponding energy bin of width 0.1.

We have determined the average and the most probable energies of the spins at low temperature for q=1. Figure 2 shows the temperature dependence of the spin wave energy, determined from the average and the most probable energies of the spins. The full lines are the least-squares fitted straight lines; y=ax. When the E_{sw} vs T is determined from the most probable energy of the spin, we obtain E_{sw}=0.47T. The coefficient of determination (R^2) in the least squares fit, was found to be 0.94. Similarly, we obtain, E_{sw}=0.59T, when we consider the average energy of the spin. In this case we obtain R^2=0.99. It is seen that the coefficients 0.47 and 0.59 are in good agreement with the theoretical value ½. This indicates that the spin waves are the dominant excitations at low temperatures.

The energy needed to create a vortex-anti-vortex pair (2μ) can be estimated from the expected exponential temperature dependence of vortex density: $V\sim e^{-2\mu/T}$. We obtained a value of 2μ=7.3. 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. 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 2μ=7.55 obtained in the simulations are in good agreement with the present results. We note here that the analytical value estimated by the BKT theory is 9.9. Since the

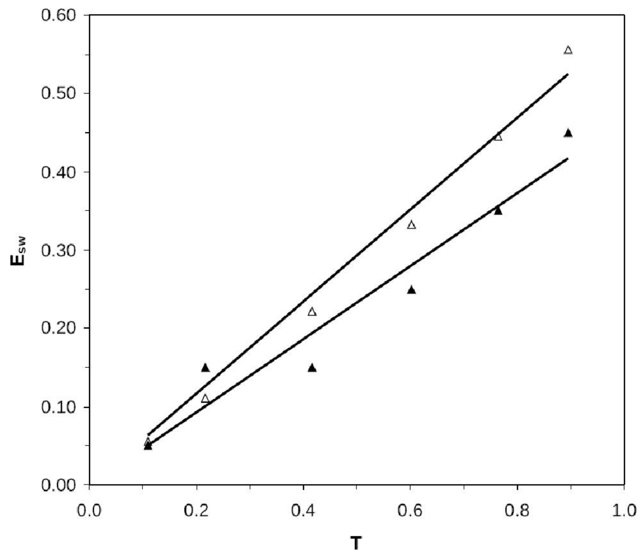

Figure 2 : The temperature dependence of spin wave energy, determined from the average (Δ) and the most probable (▲) energies of the spins. The full lines are the least-squares fitted straight lines.

vortices are of topological nature, we do not observe, any peak at large value of E_s. In this context, we note that the spin wave excitations, in equilibrium, obeys the following exponential dependence: $\sim e^{-E/kT}$. The frequency of most probable spin wave energy is seen (figure 1) to reduce with increase in temperature. From figure 3, it is seen that the vortex unbinding transition takes place, when the frequency of the most probable spin-wave energy

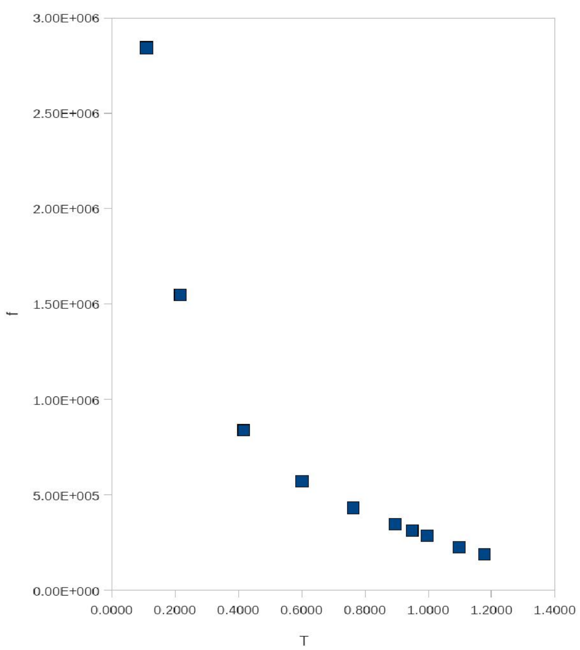

Figure 3 : The frequency of most probable spin wave energy as a function of temperature. The frequency is determined from the number of times out of the 5×10^6 MCSS that the spin is in the corresponding energy bin of width 0.1.

reduces by one order magnitude.

In conclusion, we have studied the spin waves in the 2D classical XY model using microcanonical Monte Carlo simulations. We have considered a 2D square lattice having 900 spins with periodic boundary conditions. The energy distribution of the spin, shows features that can be associated with spin wave and vortex excitations. The temperature dependence of the spin wave energy is determined from the average and the most probable energies of the spins; which is found to be in good agreement with that predicted from the spin wave theory. The vortex unbinding transition takes place, when the frequency of the most spin-wave energy reduces by one order of magnitude.

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