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Nature of lack-of-ergodicity in finite systems of two-dimensional Potts model

Abstract

Two dimensional (2D) *q*-state Potts model has been studied in microcanonical ensemble using Monte Carlo simulations. For the microcanonical Monte Carlo simulation 15x15 spin system and q = 10 state Potts model was chosen with periodic boundary condition. For large system energy the demon energy distribution is found to deviate from linearity and has the form $\exp(-\beta E_D+\gamma E_D^2)$. γ is found to be zero near the first-order transition. We suggest a possible origin of localized two level system observed in glasses.

Key Words

D. microcanonical Monte Carlo; D. Potts model; C. ergodicity.

The Potts model has been used to gain an understanding of phase transition in some well defined systems[1]. Moreover first-order phase transitions play an important role in the statistical mechanics of many physical phenomena of finite systems. In this context microcanonical Monte Carlo simulations play an important role[2]. The energy as a function of temperature for such systems shows a 'S' shape at the first-order transition. Therefore, understanding the 1st order phase transition in this microcanonical MC simulation technique has gained interest. In this communication we report the origin of the lack of ergodicity in 2D q-state Potts model[3].

The Hamiltonian of the q-state Potts model is given by

$$H=-J\Sigma_{<i,j>}\delta(\sigma_i\sigma_j) \quad (1)$$

where δ is the Kronecker delta. J is the interaction strength (> 0 for the ferromagnetic case) and the sum is over all the nearest neighbors. The spin at the ith site σ_i can take any one of the q different values. The Potts model has a first-order transition for q > 4 and a higher order transition for q≤4. The thermodynamic first-order transition temperature is given by[4]

$$k_BT_C/J=[\ln(1+\sqrt{q})]^{-1} \quad (2)$$

We consider a 2d square lattice having N × N spins with periodic boundary condition and simulated the system with N = 15 and q = 10. For q = 10 $k_BT_C/J = 0.70$. Although periodic boundary condition is used in the simulations the system is 'finite' in the sense that the 'configurations' are defined due to the updating procedure. Initially all the spins are aligned in one state (i.e., state 1). This corresponds to the lowest energy state of the system. An extra degree of freedom called the 'demon' is allowed to move from one spin site to the another sequentially on the lattice as it exchanges energy with spins changing the microstate. The simulation starts with the demon having a fixed amount of energy (E_D). This demon energy when added to the system energy (E_S) corresponds to the total energy of the system. A random number in the interval [1,q] is generated which corresponds to a possible new state of the spin. The change in energy is calculated corresponding to this change in the spin state. A positive change in energy is allowed if the demon has sufficient energy. Otherwise the old spin state is retained. A negative or zero change in energy is always accepted and the demon receives that amount of energy from the spin system. The criterion of choosing the random number and accepting the change of configuration as described above satisfies a restricted form of detailed balance. The demon here takes energy values that are integral multiples of J. In equilibrium the demon energy distribution is exponential.

$$f \sim \exp(-\beta E_D) \quad (3)$$

where $\beta = 1/k_B T$ and k_B is the Boltzmann constant. It can be shown that the the following equation is valid to determine the system temperature from the simulation.

$$k_B T = 1/\ln(1 + \langle E_D \rangle^{-1}) \quad (4)$$

(Hereafter $k_B T/J$ is replaced by T and E/J by E for simplicity). The ergodicity of this simulation has been reported earlier. In our study randomness is incorporated in the choice of the spin state. The simulation did not give an exponential distribution for E_D for small values of system energy. The situation did not change by a random choice of the spin site. This is a drawback especially for smaller system sizes as it limits how low the temperature can be when the system energy can only take discrete values. It was found that for a 10x10 spin system with q=10 state the demon can not have energy that is sufficiently small compared to the total energy $E_T(=E_S+E_d)$ when $E_S<-179$. This arises due to discrete nature of energy distribution. Examination of the spin configurations revealed that in the Potts model the fluctuation of spin is localized in small regions. An acceptable exponential distribution is obtained for $E_S>-179$ for 10x10 spin system with q=10 states. Moreover, ergodicity did not seem to depend on the value of q. It was found that at high temperatures the distribution of E_D deviated from exponential. The distribution could be fitted with the following expression.

$$\ln f = a - \beta' E_D + \gamma E_D^2 \quad (5)$$

Here β' can be associated with the 'inverse temperature' (i.e., $1/k_B T$). It is found that γ is finite at higher temperatures. As the system energy is reduced γ becomes zero near the first order transition. The variations of β' and γ with system energy per spin $E(=E_T/N^2)$ is shown in figures 1 and 2.

The cooling from higher T into the 1st order phase transition is shown in figure 1. Further cooling or at still lower temperatures the system shows lack of ergodicity. The heating and cooling curves are found to be similar for E vs β' which is seen in figure 1. However, difference in heating and cooling curves are apparent in E vs γ which is shown in figure 2. It is seen that during cooling γ changes

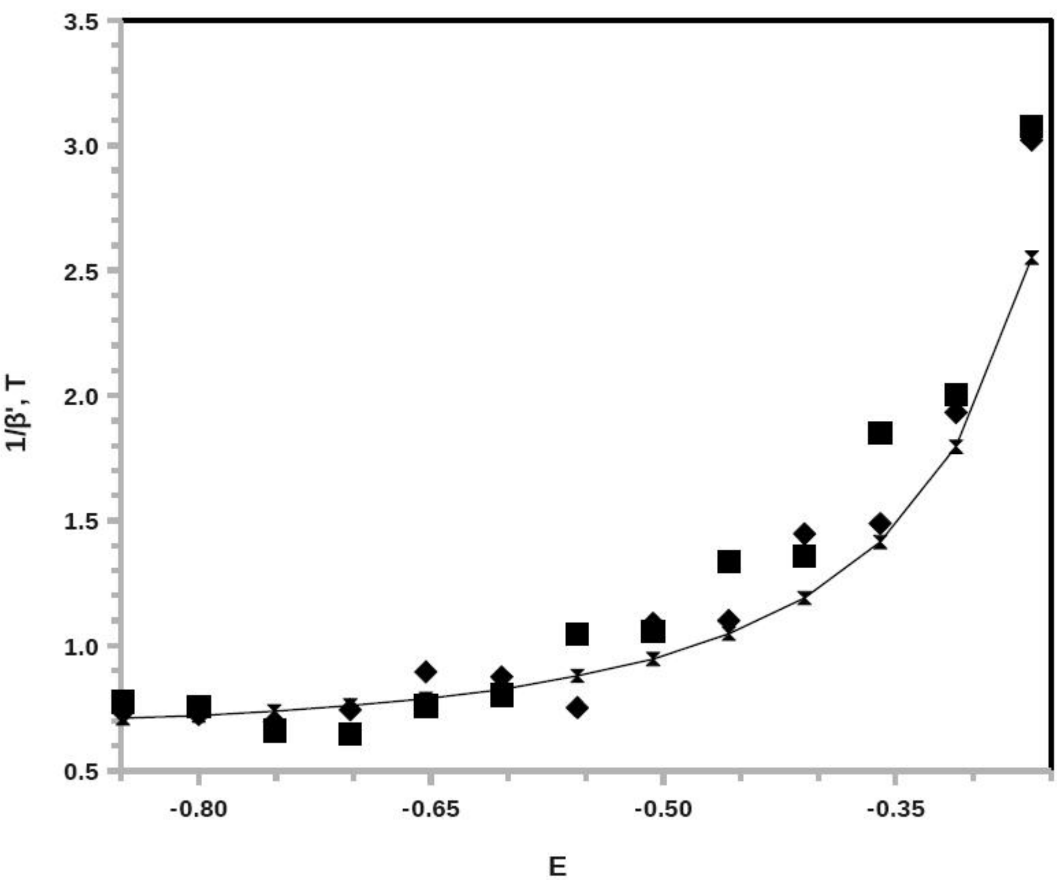

Figure 1 : 1/β' as a function of system energy per spin for cooling (■) and heating (♦). The simulation were carried out on a 15x15 q=10 state Potts model with periodic boundary conditions. Average T (⧗) of cooling and heating is shown for comparison and the solid line through the data is to guide the eye.

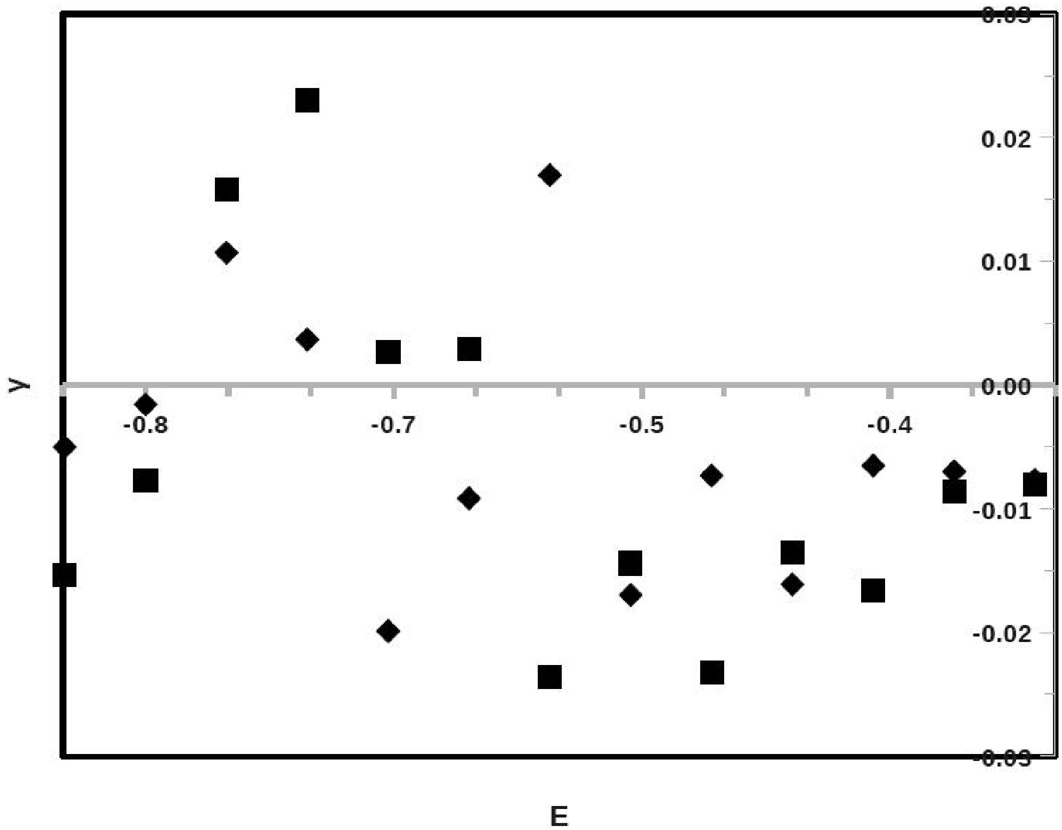

Figure 2 : γ as a function of system energy per spin for cooling (■) and heating (♦). The simulations were carried out on a 15x15 q=10 state Potts model with periodic boundary conditions. γ becomes zero near the first order transition.

sign from negative to positive and then to negative again near the 1st order transition.

Spin systems such as Heisenberg, XY and Ising models has been used in the past to understand the nature phase transitions in real magnetic systems[5]. In this context we note that finite systems of Potts model can help in understanding glass transition. Anomalous low temperature specific heat arising due to quantum mechanical tunneling in localized two-level system[6-8]. This give rise to time dependent specific heat at low temperatures[9]. Specific heat has also been found to be frequency dependent for liquids undergoing glass transitions[10,11]. In Potts model the two system energies for which γ is zero during cooling represents the 'ergodic' states. This can be related to the two-level systems observed in glasses at low temperatures.

In conclusion, nature of lack-of-ergodicity has been studied in finite systems of 2d Potts model using microcanonical Monte Carlo simulations. For large system energy the demon energy distribution is found to deviate from linearity and has the form $\exp(-\beta E_D + \gamma E_D^2)$. γ is found to be zero near the first-order transition.

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