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Microcanonical Monte Carlo simulations of the first-order transition in the two-dimensional Potts model

S B Ota† and Smita Ota‡

† Institute of Physics, Sachivalaya Marg, Bhubaneswar 751005, India
‡ Institute of Materials Science, 68/1 Laxmi Vihar, Bhubaneswar 751005, India

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Abstract. Microcanonical Monte Carlo simulations have been implemented in the two-dimensional (2D) q-state Potts model. The ergodicity of this simulation technique for the Potts model is studied. It does not seem to depend on the value of q. A lack of ergodicity for small values of the system energy is reported and discussed. It has been found that the temperature dependences of physical quantities exhibit an 'S'-shaped nature at the first-order transition. The degree of 'S'-shaped nature was enhanced by increasing q and reducing the system size. We believe on the basis of our computer simulations that the 'S' shape represents the equilibrium behaviour of a finite isolated system.

1. Introduction

Among the various computer simulation methods for the microcanonical ensemble [1–7], *the microcanonical Monte Carlo (MC) simulation technique proposed by Creutz* [8] appears to be particularly simple and fast and hence is probably the best. Here, the system energy is an input parameter and the temperature is obtained through the simulations. Among the various spin models, this microcanonical MC simulation technique has been applied to the Ising model [8–14] and the XY-model [15–17]. Ergodicity has been demonstrated empirically for these models [10, 15]. The system complexity is expected to give rise to ergodicity. Some degree of randomness is generally incorporated in the simulation procedure, which helps in achieving ergodicity. Renormalization-group calculations [18–20] have also been added to this technique conveniently [21]. The full potential of this technique is yet to be explored in connection with various statistical systems and situations.

In this paper, we study the first-order transition within the finite-size two-dimensional (2D) *q-state Potts model* [22, 23] and establish the ergodicity of this technique by comparing with exact results. This study is also motivated by the fact that the Potts model undergoes a well studied first-order transition and provides a system of increasing complexity as q increases. Therefore, one can study the role of system complexity in achieving ergodicity, and here we specify what one means by system complexity in this particular method of microcanonical MC simulation [8].

The Potts model has been used to gain an understanding of the phase transitions in some well defined compounds. Moreover, first-order phase transitions play an important role in the *statistical mechanics* of many physical phenomena of *finite systems*—such as the evolution of the early universe, fragmenting nuclei, fragmenting atomic clusters and melting phase transitions in van der Waals clusters: in this context, microcanonical simulations play an

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important role. In the past, considerable efforts have been made to develop refined numerical methods for their description [24–36]. The energy as a function of temperature for such systems shows an 'S' shape at the first-order transition. Therefore, the applicability of this microcanonical MC simulation technique to such situations is also explored.

It is also well known that metastability gives rise to an 'S' shape [37]. For instance, it arises in weak-long-range-force models. In the limit of infinite interaction range, the free-energy cost of a change in the equilibrium state is extensive, as a function of the system volume, and mean-field approximation predicts that metastability lifetimes are infinite in the thermodynamic limit. However, in the context of this paper, we have not considered such situations, for convenience.

The paper is organized as follows. In section 2, we describe the simulation procedure. The ergodicity in the computer simulations is discussed in section 3. The results are given in section 4. In section 5, we examine the coexistence region. The conclusions are presented in section 6.

2. The simulation procedure

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

$$H = -J \sum_{(i,j)} \delta(\sigma_i \sigma_j) \tag{1}$$

where δ is the Kronecker delta, J is the interaction strength (>0 for the ferromagnetic case) and the sum is over all the nearest neighbours. 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 $q \leqslant 4$.

We considered a 2D square lattice having 100, 225, 400, 900 or 3600 spins with periodic boundary conditions and simulated these systems with different values of $q > 4$ (i.e., $q = 10$, 20 and 30). 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 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 at the lowest desired temperature. 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 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 [8]. The demon here takes energy values that are integral multiples of J. Therefore, we find the following equation, valid for the Potts model, to determine the system temperature from the average demon energy [8, 14]:

$$k_B T = 1/\ln(1 + \langle E_d \rangle^{-1}) \tag{2}$$

where k_B is the Boltzmann constant. (Hereafter we replace $k_B T/J$ by T and E/J by E for simplicity.) Following Challa, Landau and Binder [25] we define the order parameter, m, as follows:

$$m = [q(N_{max}/N) - 1]/(q - 1) \tag{3}$$

where: N_1 is the number of spins in state 1, N_2 is the number in state 2 etc; N_{max} is the maximum of $N_1, N_2, \ldots, N_q$; and N is the total number of spins.

The equilibration and the nature of the fluctuation of the order parameter with this algorithm are shown in figure 1. From this figure it is evident that 1×10^5 MC steps per spin (MCSS) are sufficient for equilibration and averaging of the physical quantities. We, however, use 4×10^5 MCSS for equilibration and 4×10^5 MCSS for averaging for a 60×60 spin system. The physical quantities calculated after each MCSS were used for the averaging. The simulations were each constituted of a heating run followed by a cooling one. During the heating (cooling) cycle, energy was added (subtracted) to (from) the spin system through the demon. The difference between the results for the heating and cooling runs was typically less than one per cent. The physical quantities computed are averages of those for the heating and cooling runs. The standard deviation for the temperature is typically around one per cent. In the next section, we study the ergodicity of this simulation technique.

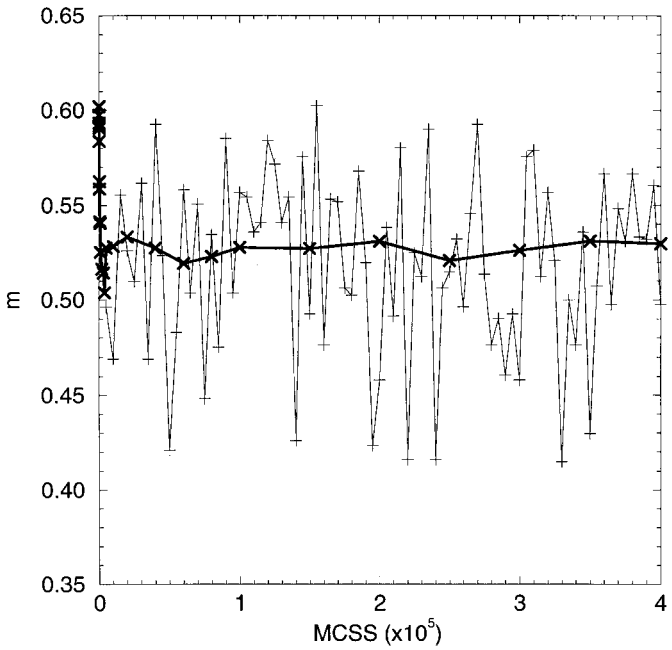

Figure 1. The order parameter as a function of the number of MCSS for the $q = 10$-state Potts model on a 30×30 lattice. The initial configuration was with all spins in state 1. The corresponding system energy is -1150 and the temperature is 0.703. The bold curve shows the equilibration. Each point on this curve represents an average over all configurations starting from the first MCSS up to a given MCSS. The light curve represents the instantaneous values of m plotted after every 5000 MCSS, showing the fluctuations.

3. The ergodicity

In equilibrium, the demon energy was found to be approximately distributed according to Boltzmann's law. In this context, the recent study of Cruz *et al* [6] of the local microcanonical over-relaxation (LMO) technique is of interest. They found that the LMO technique can lack ergodicity when the updating is *sequential* and becomes ergodic when the updating is *random*. In our study, the randomness is incorporated in the choice of the spin state. The simulations,

however, did not give an exponential distribution of E_d for small values of the system energy. A *random* choice of the spin site also does not help the situation. This is illustrated in figure 2. 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. For small values of the system energy, there are fewer energy states accessible to the demon (figure 2). In order to determine the energy value above which the distribution is exponential, we studied the nature of the demon energy distribution as a function of system energy. To this end, we have calculated $\chi^2/(n-2)$ for the least-squares straight-line fitting of $\ln(f)$ versus E_d for different system energies (-194 to -165 units) for a 10×10 spin system with $q = 10$ states. This is displayed in figure 3. Here, n corresponds to the number of points used for the least-squares fitting for which $f > 100$. It is seen in figure 3 that $\chi^2/(n-2)$ reduces to an acceptable value for system energies greater than -179.

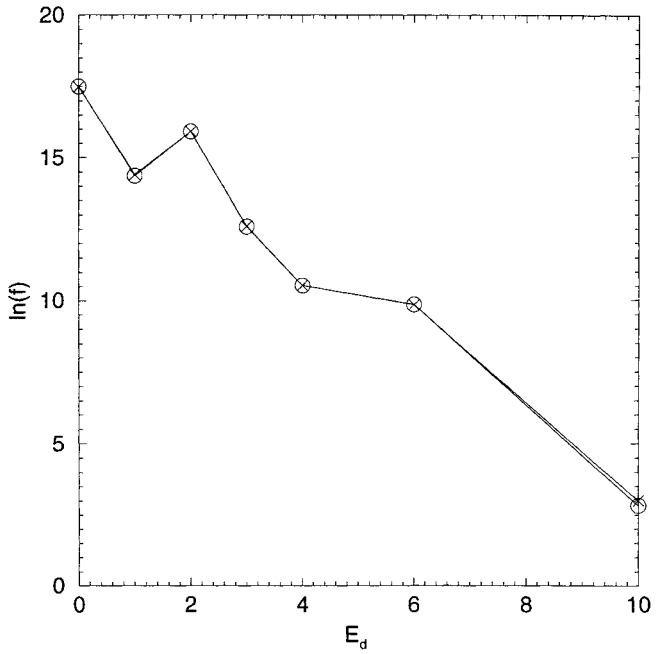

Figure 2. The distribution of demon energies over 5×10^5 MCSS after the 5×10^5 MCSS used for the equilibration for sequential updating (◯) and random updating (×). The simulations are carried out on a 10×10 spin system with $q = 10$ states. The ordinate represents the natural logarithm of the number of times out of 5×10^7 steps that the demon is at the corresponding energy of 0, J, $2J$, $3J$, $4J$, $6J$ and $10J$. The total energy is -190. Note that the lowest total energy is -200. The straight lines connecting the data points are to guide the eye.

One can understand this as follows. For system energies smaller than -179, the demon cannot have energy that is sufficiently small compared to the total energy E_T ($=E_s + E_d$) [8] due to the discrete symmetry of the model. Therefore, one does not obtain an exponential distribution of E_d. However, such a situation does not arise in models with continuous symmetry [15] such as the XY-model [38–48]. One can also look at the situation from a different point of view. In the microcanonical MC simulations, the system acts as a heat bath for an individual spin. However, examination of the spin configurations revealed that in the Potts model the spin fluctuation is localized in small regions and the system cannot act as a heat bath. Therefore, ergodicity is not obtained. In contrast, for the XY-model, the spin fluctuation

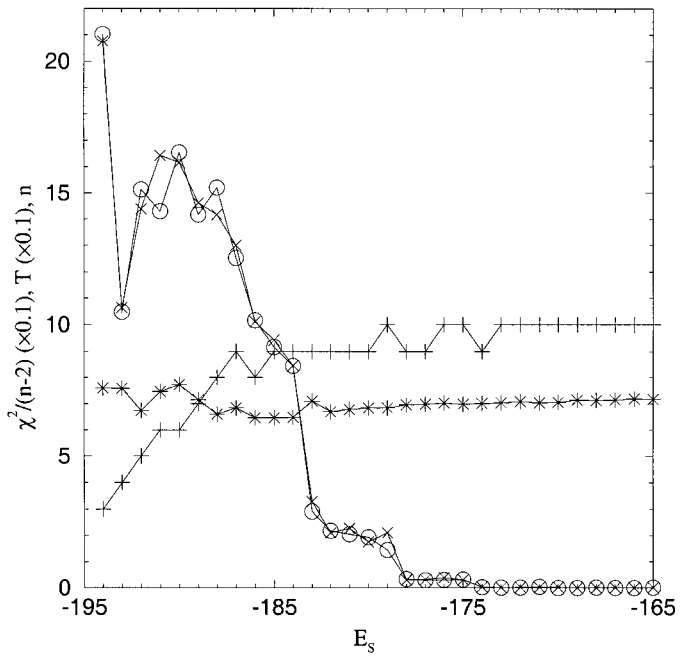

Figure 3. $\chi^2/(n-2)$ ($\times$), T ($\star$) and n (+) as functions of system energy for random updating of the spins. The ◯ represent $\chi^2/(n-2)$ for sequential updating of the spins. Here, 5×10^5 MCSS for equilibration with 5×10^5 MCSS for averaging of the data were used for the simulations. The simulations are carried out on a 10×10 spin system with $q = 10$ states. It may be noted that the ground-state energy is -200 units. The straight lines connecting the data points are to guide the eye. An acceptable exponential distribution is obtained for system energy above -179. This corresponds to a number of independent accessible energy states of the system of about 20. It is seen from the figure that the ergodicity does not differ noticeably for random and sequential updating.

is dissipated over the entire spin system and the system can still act as a heat bath even for small values of system energies. In order to check this situation, we simulated the 2D classical XY-model having 30×30 spins using the present microcanonical MC simulation technique. We used a total energy of $E_T = 5$, above the ground state ($E_T = 0$), which corresponds to a temperature of 0.011. Examination of the spin configurations confirmed smooth dissipation of the spin fluctuation in the 2D XY-model. The demon energy distribution was found to be exponential for E_d up to about 0.12 (figure 4). The *ergodicity* was found to be excellent for the 2D XY-model [15, 17].

Next we try to understand what determines the ergodicity. For this purpose, we examine how the ergodicity depends on q. As before, we calculated $\chi^2/(n-2)$ as a function of system energy for different values of q. The simulations were carried out on a 10×10 spin system for $q = 10$, 30 and 50. It is seen that the ergodicity does not seem to depend on the value of q (figure 5). The reason behind this may be that, although the number of accessible states (or spin configurations) increases with q for a given E_s, the number of independent accessible *energy* states does not change with q for E_d and E_s in combination. Therefore, the measure of system complexity which generates the ergodicity is the number of accessible *energy* states. In section 4, we compare the present microcanonical MC simulation results with the exact results.

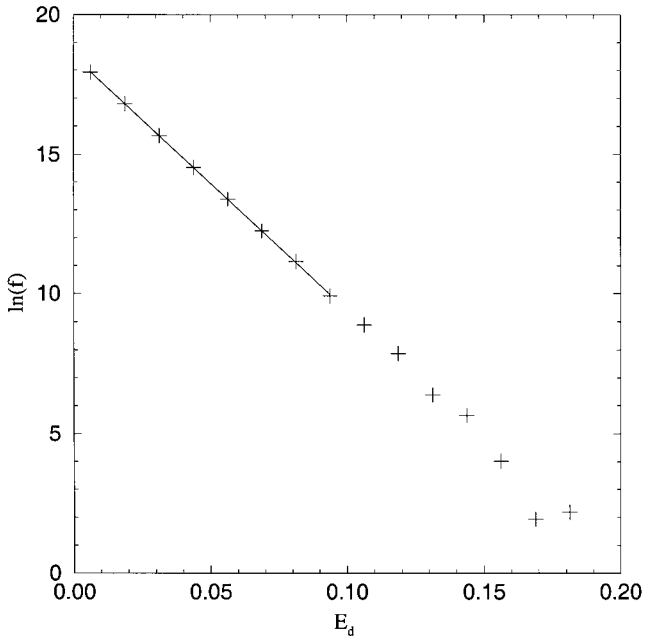

Figure 4. The distribution of demon energies over 1×10^5 MCSS after the 1×10^5 MCSS used for the equilibration for the 2D XY-model. The simulations are carried out on a 30×30 spin system with periodic boundary conditions. The initial configuration was with all spins parallel to each other. The ordinate represents the natural logarithm of the number of times out of the 9×10^7 steps that the demon is in the corresponding energy bin of width 0.0125. The straight line represents the least-squares fitting of the exponential distribution, giving a temperature of 0.011.

4. Results

Figures 6 and 7 display the temperature dependences of the total energy per spin and average order parameter, respectively. The transition region is seen to be 'S' shaped in nature. We define the middle of the two extrema in the 'S'-shaped region as the transition temperature. We observed that T_c increases on reducing the system size, which is probably to be expected from finite-size scaling theory [26, 49–51]. We found that the first-order transition occurs at $T_c = 0.701$, 0.589 and 0.536 for $q = 10$, 20 and 30, respectively, for a 30×30 spin system. This can be compared with the exact values of $T_c = 0.7012$, 0.5883 and 0.5352 for $q = 10$, 20 and 30, respectively, which are obtained from Baxter's formula [52]:

$$k_B T_c/J = [\ln(1+\sqrt{q})]^{-1}. \tag{4}$$

Baxter [52] has given an exact expression for the latent heat:

$$(E_+ - E_-)/J = 2(1+1/\sqrt{q})\tanh(\theta/2)\prod_{n=1}^{\infty}[\tanh(n\theta)]^2 \tag{5}$$

where $2\cosh\theta = \sqrt{q}$. One can determine E_+ and E_- using equation (5) together with the expression given by Kihara, Midzuno and Shizume [53]:

$$(E_+ + E_-)/2J = -[1+1/\sqrt{q}]. \tag{6}$$

The values of E_+ (E_-) are -0.9682 (-1.6643), -0.6265 (-1.8207) and -0.4874 (-1.8778) for $q = 10$, 20 and 30, respectively. The exact result for the order parameter discontinuity at

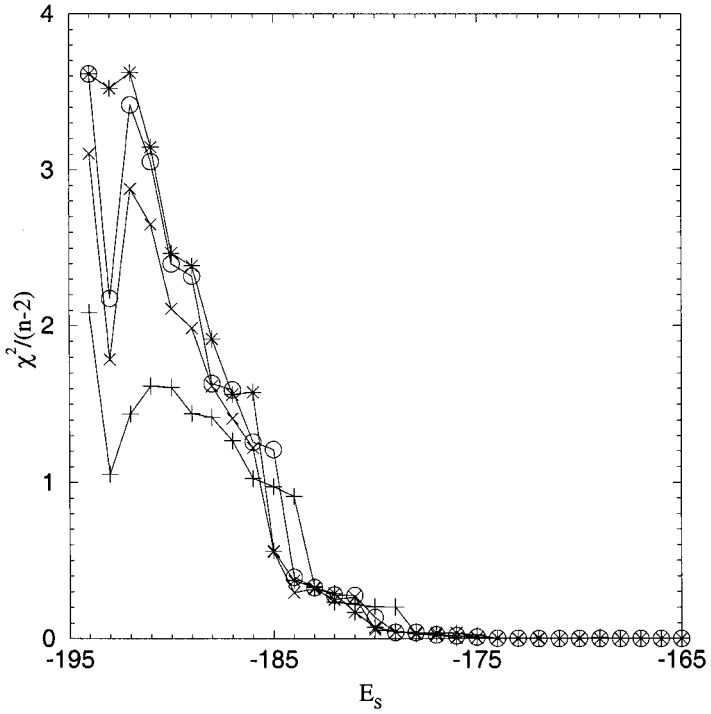

Figure 5. $\chi^2/(n-2)$ as a function of system energy for $q = 10$ (+), $q = 30$ ($\times$) and $q = 50$ ($\star$) over 5×10^5 MCSS after the 5×10^5 MCSS used for the equilibration. The $\bigcirc$ represent $q = 50$ over 2.5×10^6 MCSS after the 2.5×10^6 MCSS used for the equilibration. The ergodicity does not seem to depend on q. It may be noted that the ground-state energy of a 10×10 spin system is -200 units. The straight lines connecting the data points are to guide the eye. Random updating was used for these simulations.

T_c is given by [54, 55]

$$\Delta m = 1 - q^{-1} - 3q^{-2} - 9q^{-3} - 27q^{-4} - \cdots. \tag{7}$$

The values of Δm for $q = 10$, 20 and 30 are 0.8571, 0.9412 and 0.9630, respectively. The values of E_+, E_- and Δm are marked in figures 6 and 7 for comparison, and agree very well with the exact results.

5. The coexistence region

In this section, we examine the 'S' shape of the coexistence region observed in the simulations. Harris [12] has studied the first-order transition in an Ising-like system using the microcanonical MC simulations of Creutz and has also observed a similar shape. We estimated the width of the transition (δT_c) as the temperature difference between the two extrema of the 'S'-shaped region. We have found that δT_c increases on increasing q and on reducing the system size. For instance, δT_c increased from 0.020 to 0.035 as q was increased from 10 to 30 for a 30×30 spin system. For a fixed q ($q = 10$), δT_c was also found to increase from 0.011 to 0.038 as the system size was reduced from 60×60 to 10×10. We studied the coexistence region further for possible effects due to *metastability* by increasing the number of MCSS for equilibration and averaging. To this end, a comparison of the computed value of $\langle T \rangle$ has been

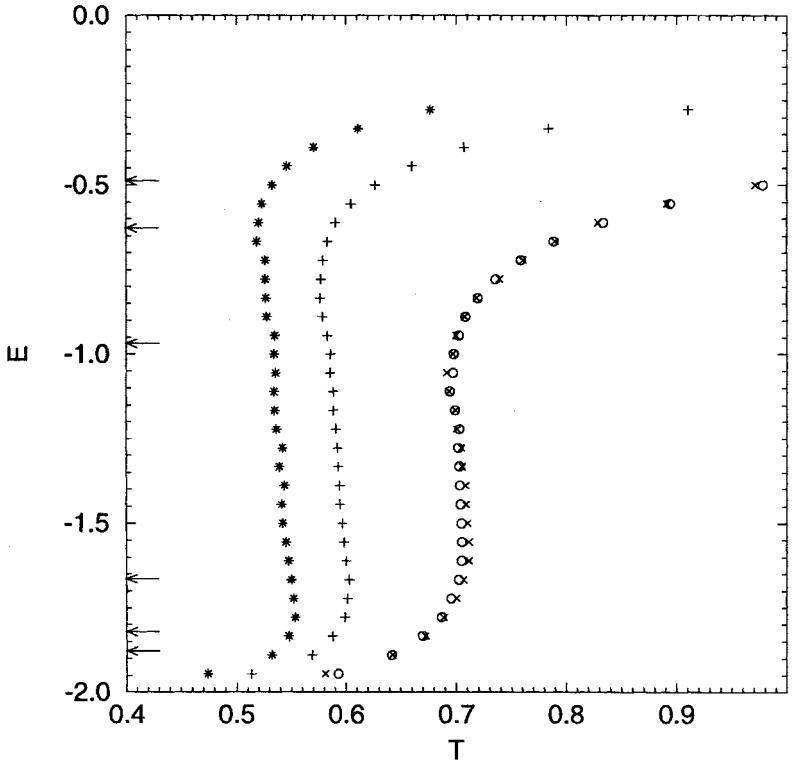

Figure 6. The temperature dependence of the total energy per spin for $q = 10$ (×), 20 (+) and 30 (⋆) states of a 30×30 spin system and $q = 10$ states (◯) of a 60×60 spin system. The exact values of E_+ and E_- are marked on the y-axis. The lower set of arrows are for $q = 10$; the middle set are for $q = 20$; the upper set are for $q = 30$.

carried out for a 10×10 spin system by simulating it over 2×10^5 and 1×10^6 MCSS. The ensemble averages of the temperatures and δT_c were found to have *almost the same* values even after increasing the number of MCSS significantly.

The 'S'-shaped nature of the coexistence region of a first-order transition for a finite system has been observed in microcanonical molecular dynamics simulations [56–59] and microcanonical MC simulations [36, 60]. We have also simulated the first-order transition in the 2D extended XY-model [61] using the present microcanonical MC simulation technique and have also obtained the 'S' shape [16]. (It has been noted [60] that in the molecular dynamics simulations of Jellinek *et al* [62], the 'S' shape disappears when long-time averages are taken.) In contrast, the canonical MC simulations give rise to a smearing of the coexistence region for models with discrete symmetry [24–26] and with continuous symmetry [61, 63]. The canonical Monte Carlo simulations do not probe correctly the transition region of a first-order transition, because the temperature is predefined. The microcanonical MC simulations probe the coexistence region of the first-order transition correctly [16]. Therefore, the question arises of whether the 'S' shape represents the equilibrium behaviour or not. We note here that system is definitely finite in the present simulations, although a periodic boundary condition has been used to mimic an infinite system. We believe from our computer simulations that *the 'S' shape does represent the equilibrium behaviour of a finite isolated system.*

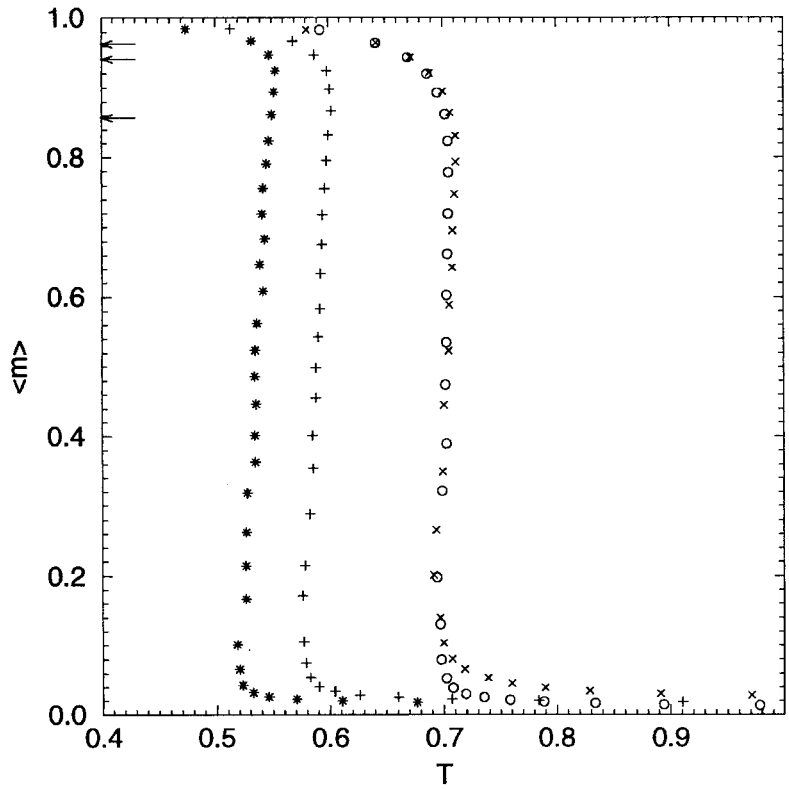

Figure 7. The temperature dependence of the average order parameter for $q = 10$ ($\times$), 20 (+) and 30 ($\star$) states of a 30×30 spin system and $q = 10$ states ($\bigcirc$) of a 60×60 spin system. The exact values of Δm are marked on the y-axis. The lower arrow is for $q = 10$; the middle arrow is for $q = 20$; the upper arrow is for $q = 30$.

6. Conclusions

In conclusion, we have carried out microcanonical MC simulations on the 2D q-state Potts model. The ergodicity of this technique for this model is studied. It does not seem to depend on the value of q. A lack of ergodicity, which occurs in a particular situation, when the system energy is discrete as a function of temperature, is reported and discussed. This occurs only for small values of the system energy. This is a drawback, especially when the system size is small, as it limits how low the temperature can be. It has been found that the temperature dependences of the physical quantities exhibit 'S'-shaped natures at the first-order transition. The degree of 'S'-shaped nature was enhanced by increasing q and reducing the system size. We explain here that the 'S' shape observed in microcanonical MC simulations is the equilibrium behaviour of a finite isolated system exhibiting a first-order transition. This study is different from that of the 'spinodal', which is associated with the kinetics of a system.

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