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1988 J. Phys. A: Math. Gen. 21 769

(http://iopscience.iop.org/0305-4470/21/3/032)

J. Phys. A: Math. Gen. **21** (1988) 769-772. Printed in the UK

Critical relaxation of the two-dimensional three-state Potts model with conserved dynamics

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Received 30 June 1987, in final form 8 October 1987

Abstract. The dynamical critical exponent z is obtained using the finite-size scaling method for the two-dimensional three-state Potts model with conserved dynamics. It is observed that there is a change in the dynamical behaviour of the system at the size $n = 15$. For finite lattices of sizes $n \leqslant 15$, the value of z is predicted as $z = 2.0 \pm 0.1$. For $n \geqslant 15$, the asymptotic behaviour is observed and z is calculated as $z = 2.78 \pm 0.20$.

1. Introduction

Studies on the dynamics of the two-dimensional three-state Potts model have resulted in a range of different values of the dynamical critical exponent z. Forgacs *et al* (1980) obtained a value of $z = 2.25$ using a Migdal type of recursion method. Binder (1981) calculated the non-linear exponent Δ^{nl} as $\Delta^{nl} = 1.9$ through a Monte Carlo simulation using dynamical scaling and found that Δ^{nl} is independent of the number of states. His result corresponds to a z value of $z = 2.41$ from the relation $z = (\Delta^{nl} + \beta)/\nu$. Tobochnik and Jayaprakash (1982) used a dynamic Monte Carlo simulation method to obtain z. Their result is $z = 2.7 \pm 0.4$. Aydın and Yalabık (1984) calculated z using a dynamic Monte Carlo renormalisation group method. They found exactly the same value as obtained by Tobochnik and Jayaprakash. Later, Aydın and Yalabık (1985) used the finite-size scaling method to find z. They obtained $z = 2.2 \pm 0.1$. Domany (1984) predicted a value for z of 2.8 through the relation $z\nu = 2 + \alpha$ which is obtained using hyperscaling.

Recently, Lage (1986) calculated z as $z = 2.53$ for the two-dimensional three-state Potts model using a dynamical theory which includes a decimation procedure. De Arcangelis and Jan (1986) found a value for z, $z = 2.43 \pm 0.15$. They used a dynamic Monte Carlo renormalisation group method with Glauber dynamics. Tang and Landau (1986) calculated the non-linear exponent as $\Delta^{nl} = 2.1$ and they found that Δ^{nl} is independent of the number of states. Their result is consistent with the value obtained by Binder (1981). Lage (1987) studied critical dynamics of general q-state Potts models on d-dimensional hypercubic lattices. He used a simple bond moving technique, followed by a decimation, and obtained $z = 2.76$ for $d = 2$ and $q = 3$.

In the present study, the dynamical critical exponent z is calculated for the two-dimensional three-state Potts model. To our knowledge, this is the first study of this model using conserved dynamics. The finite-size scaling method is used to obtain the relaxation times for system sizes $n = 3, 6, \ldots, 21$. The value of z is calculated as $z = 2.78 \pm 0.20$ for sizes $n \geqslant 15$. A prediction is made for $n \leqslant 15$. The result is $z = 2.0 \pm 0.1$.

0305-4470/88/030769+04$02.50

The layout of this paper is as follows. In § 2, the method and procedure are described. The results and discussions are given in § 3.

2. The method and procedure

The Potts model can be defined through the Hamiltonian H of the form

$$-\frac{H}{KT} = K \sum_{\langle ij \rangle} \delta_{S_i,S_j} \qquad S_i = 1, 2, 3 \tag{1}$$

where the summation is over all nearest-neighbour sites, k is the Boltzmann constant, T is the temperature and S_i represents spin variables on a lattice. K corresponds to the nearest-neighbour coupling and has a critical value K_c, $K_c = \ln(1+\sqrt{3})$ which is an exact result (Potts 1952).

The asymptotic behaviour of a finite-size system (at the critical temperature of the infinite system) can be shown by the relation (Suzuki 1977)

$$\tau \sim n^z \tag{2}$$

where τ is the relaxation time, n is the size of the system and z is the dynamical critical exponent. For small sizes, at which the asymptotic behaviour cannot be reached, the free energy expression with a correction term (Barber 1983) can be used to describe the behaviour of the system. In the case of dynamical scaling, equation (2) is expected to have the form

$$\tau \sim n^z(1 + an^{-\phi}) \tag{3}$$

for small system sizes. Here ϕ is the correction to scaling exponent and a is a constant.

The finite-size scaling method (Aydın and Yalabık 1985) is used to obtain the relaxation times for different system sizes. A random-spin configuration is generated initially and the system is relaxed to equilibrium through a standard Monte Carlo procedure (Binder 1981). Time is measured in Monte Carlo steps (MCS). The order parameter is conserved by exchanging the spin states of two nearest-neighbour sites if the new configuration corresponds to lower energy. In this manner, the total number of each of the three states in the lattice is conserved locally and globally. The absorption of atoms on some surfaces can be described by the two-dimensional three-state Potts model (see for example the study by Berker (1978)). The conserved dynamics is an example of the chemisorption of atoms on surfaces.

The relaxation times are calculated using the average time-dependent correlation functions which can be obtained from the relation

$$C(t) = \langle S_i(t+t')S_j(t') \rangle \tag{4}$$

where the average is taken over t' and the spin sites i, j. S_i and S_j correspond either to neighbouring spins (nearest-neighbour correlation) or to the same spin (self-correlation). $C(t)$ is calculated for square lattices of sizes $n = 3, 6, \ldots, 21$. At sufficiently long times, $C(t)$ is expected to relax with the largest time constant τ of the system. τ can be evaluated using the time variation of $C(t)$ for each size.

The relaxation time values (τ) and the total time (in MCS) elapsed to reach the equilibrium for different system sizes are given in table 1. Figure 1 shows the log–log plot of τ as a function of n. For sizes $n \leqslant 15$, the system exhibits a non-asymptotic beahviour, as can be seen from figure 1. Through a fitting procedure, a prediction is

Table 1. The relaxation time values (τ) calculated and the total time (in MCS) elapsed to reach the equilibrium for system sizes $n = 3, 6, \ldots, 21$.

n	τ	Total number of MCS	Number of independent runs
3	1.27	16×10^5	1
6	2.50	6×10^5	2
9	3.68	12×10^5	3
12	4.73	$\sim 7 \times 10^5$	2
15	6.35	$\sim 4 \times 10^5$	3
18	10.40	7×10^5	4
21	16.21 ± 4.14	$\sim 4 \times 10^5$	1

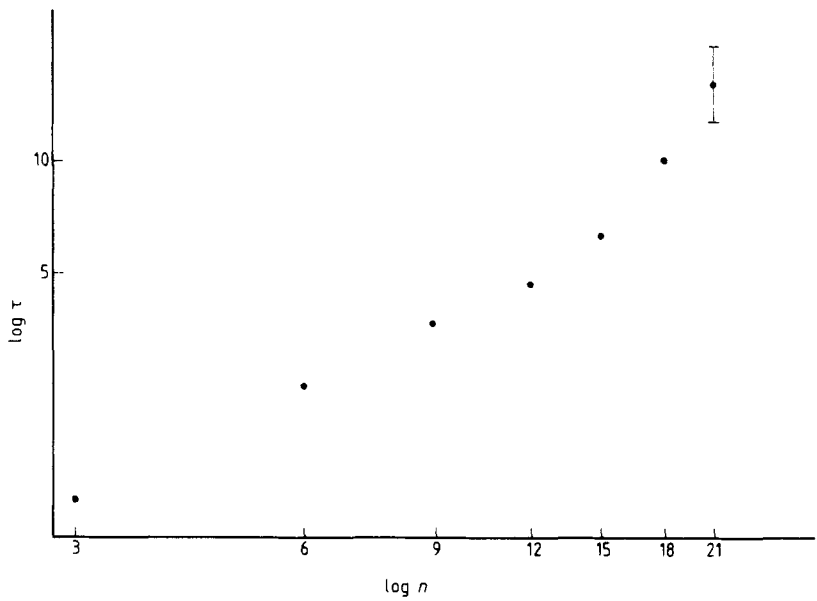

Figure 1. The log-log plot of τ as a function of n.

made for the value of z and the correction to scaling exponent ϕ using equation (3). The results are $z = 2.0 \pm 0.1$ and $\phi = 0.79 \pm 0.16$. When the sizes $n = 18$ and $n = 21$ are included in this calculation, it is not possible to obtain a set of z and ϕ values. For these sizes, the data points in figure 1 have a tendency to lie on a line including the size $n = 15$. Hence z is calculated using the asymptotic relation (equation (2)) for $n \geqslant 15$. The result is $z = 2.78 \pm 0.20$. For sizes $n \geqslant 15$, the second term in equation (3) is expected to be negligibly small. In fact, use of equation (3) (to check the validity of equation (2) for these sizes) gives the same result with the best fit values $z = 2.785$ and $\phi = 0$.

3. Results and discussions

In the present study, the value of the dynamical critical exponent z is calculated for the two-dimensional three-state Potts model with conserved dynamics. Two different

values are obtained depending on the size of the system. The value $z = 2.78 \pm 0.20$ for system sizes $n \geq 15$ is consistent with the results of Tobochnik and Jayaprakash (1982), Aydın and Yalabık (1984), Domany (1984) and Lage (1987). The value $z = 2.0 \pm 0.1$ for $n \leq 15$ is consistent with the results of the studies by Forgacs *et al* (1980) and Aydın and Yalabık (1985).

The models having non-conserved and conserved order parameters show different behaviours in time variations of self- and nearest-neighbour correlations. When the same method was used for the model having non-conserved order parameter (Aydın and Yalabık 1985), self- and nearest-neighbour correlations showed the same time variations for sizes $n = 2, 3, \ldots, 7, 10, 16$. The asymptotic behaviour was observed and z was obtained using equation (2). In the conserved case, the relaxation times are much smaller than those of the non-conserved model and the self- and nearest-neighbour correlations have different time variations. Nevertheless, they result in the same z value. When the conserved order parameter is used, the asymptotic behaviour cannot be reached for sizes $n \leq 15$, hence z is obtained using equation (3) instead of equation (2). The Ising behaviour is observed in both models for the sizes $n \leq 15$.

The errors in τ values for sizes $n < 21$ are negligibly small since the computations are carried out in a large number of MCS compared to the relaxation times and several independent runs are made for each size. Because of the limits imposed by available computer facilities, the relaxation time for the size $n = 21$ cannot be obtained with an accuracy comparable to the accuracies achieved for the other sizes. The error in z value, $z = 2.0 \pm 0.1$, may be due to the errors arising from the fitting procedure, while the error in the value $z = 2.78 \pm 0.20$ is mainly due to the error in the relaxation time for the size $n = 21$. For sizes $n \geq 15$, one should go to larger lattices to obtain a reliable value for z using equation (2).

Acknowledgment

The authors would like to thank the Middle East Technical University Computer Center for their cooperation.

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