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1993 J. Phys. A: Math. Gen. 26 4907

(http://iopscience.iop.org/0305-4470/26/19/022)

J. Phys. A: Math. Gen. 26 (1993) 4907–4910. Printed in the UK

Numerical determination of the order of phase transition of the two-dimensional Potts model with multispin interactions

Guo-Ming Zhang† and Chuan-Zhang Yang‡

† Department of Physics, SuZhou University, SuZhou, 215006, People's Republic of China

‡ CCAST (World Laboratory) P.O. Box 8730, Beijing, 100080, People's Republic of China and Department of Physics, SuZhou University, SuZhou, 215006, People's Republic of China

Received 20 October 1992, in final form 1 June 1993

Abstract. The method of the fourth-order cumulant of energy is used together with the Monte Carlo histogram technique to study the order of phase transition of the two-dimensional Potts model with m-spin interactions in the horizontal direction and n-spin interactions in the vertical direction.

1. Introduction

The two-dimensional Potts model with multispin interactions we study in this paper was originally introduced by Turban [1] and then investigated by Alcaraz [2]. The model is defined by the Hamiltonian [1, 2]:

$$-\beta H=\sum_{L_x} K_x\left[\delta_q\left(\sum_{\mu=1}^{m}\sigma_\mu\right)\right]+\sum_{L_y} k_y\left[\delta_q\left(\sum_{\nu=1}^{n}\sigma_\nu\right)\right]$$

where k_x (k_y) is the spatial (temporal) coupling. The first sum runs over the multiple links L_x joining m successive spins in the spatial direction, the second one is over the multiple links L_y joining n successive spins in the temporal direction. The Potts variable $\{\sigma\}$ lie on the sites of the rectangular lattice and may stay in any one of the q-states $\sigma=0, 1, \ldots, (q-1)$. δ_q is a Kronecker δ function modulo q. The model is self-dual for any m and n and as long as it has a single transition the critical point will be located at the self-dual point which is given by the known relation $K_c=\ln(\sqrt{q}+1)$ for the isotropic case $k_x=k_y$. the main interest of this model lies in the change in the nature of the transition from second to first order as m and n are increased once q is fixed. Turban [1] predicted that the model has a first-order transition when m, n or q are large enough. So there is a line in the (q, m) plane where the latent heat vanishes, separating first order from second-order regions. For $q=2$, $n=2$ and any m, finite size scaling [3] and Monte Carlo methods [2–4] showed that this line went through the point $(q=2, m=3)$. Blöte [5] has shown the equivalence between $q=2$, $m=3$, $n=2$ and $q=4$, $m=n=2$ in the extreme anisotropic limit. However, this issue was not totally settled in a definite way for $q=3$. The purpose of this paper is try to locate the borderline between second-order and first-order transition for the model when $q=3$.

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Because when $m=n=2$ $q=3$, the transition is already known to be of second order [6], we will fix $n=2$ and increase m to see for which m the transition becomes first order. Our result is that when $m=3$ the model undergoes first-order transition which is in agreement with [2] by detecting quite clearly the energy differences between the two phases.

The method we used to distinguish between first and second-order transition is the cumulant technique which was proposed by K Binder [7]. This method has been used recently to locate the boderline for this model when $q=2$ [4].

Binder's fourth-order cumulant of energy is defined by

$$V_4(L)=1-\langle E^4\rangle_L/(3\langle E^2\rangle_L^2)$$

and was introduced as a quantity which could distinguish between first and second-order transition since it has a non-trivial value at a first-order transition. In either a disordered or ordered phase, $T\neq T_c$, $V_4(L)=\frac{2}{3}$ in the thermodynamic limit but at T_c, all phases contribute to $V_4(L)$, so it will have a minimum value which in the thermodynamic limit is given by [8–10]

$$V_4(L)|_{\min}=2/3-(e_1/e_2-e_2/e_1)^2/12$$

where e_1 and e_2 are the energy of the two phases at the transition temperature, while at a second-order phase transition it tends to $\frac{2}{3}$ in the thermodynamic limit for any temperature at and around the transition.

We employed the standard single-spin-flip Metropolis [11] Monte Carlo algorithm and study system with dimension $L\times L$ and periodic boundary conditions applied in all directions. We performed the simulations at the self-dual symmetrical point for the isotropic case $K_x=K_y=K_c$.

In order to locate the position and value of the minimum of the fourth-order cumulant quickly and accurately, we used the histogram method of Ferrenberg and Swendsen [12] for calculating the probability distribution of the internal energy at values of the coupling shifted from that of the actual value used in the simulation. Once in possession of the histogram the average of $\langle E^2\rangle_L$ and $\langle E^4\rangle_L$ of size L can be calculated easily. So the fourth-order cumulant of energy can be calculated easily.

With their method, it is possible to obtain complete thermodynamic information over the entire scaling region near the phase transition from a simulation at a single value of coupling in the region, and thereby, to accurately locate the positions and values of Binder's fourth-order cumulant.

Typical runs were $(5.0–7.0)\times 10^5$ Monte Carlo steps per spin (MCS). Thermalization was assumed after looking at the correlation times, which led to discarding the initial $(1–5)\times 10^4$ MCS. All the simulations were performed on Taijing 2230 at the Computer Center of SuZhou University. One of our largest series of measurements on a 48×48 lattice, MCS = 600 000, took about 60 h of CPU time.

The temperature variation of $V_4(L)$ is shown for various lattice sizes in figure 1. As the lattice size increases, the positions of the minima of the fourth-order cumulant shift to the lower temperature direction and the values of the cumulant increase. These values of the minima were fitted using a power law as suggested by finite size scaling of the form [8, 9]

$$V_L=V_\infty(1-aL^{-b}).$$

The best value obtained for V_∞ characterizes the order of the transition to be of first-order when $m=3$, $n=2$ for $q=3$, because $V_\infty=0.655\neq\frac{2}{3}$. The value of b and a

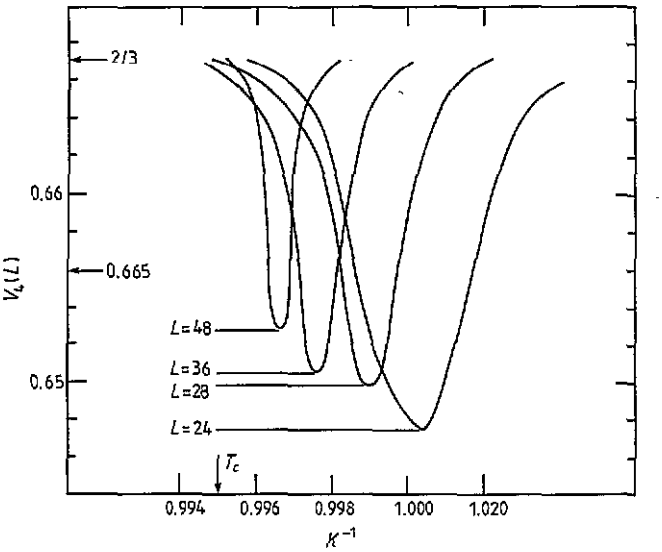

Figure 1. Temperature variation of $V_4(L)$ for various lattice sizes. The transition temperature and the trivial ($\frac{2}{3}$) and non-trivial (0.655) limits for $V_4(L)|_{\min}$ are indicated. Data for some of the lattice sizes have been omitted in order to preserve the clarity of the figure.

obtained by our fitting procedure is 1.98 and 7.035, respectively.

The transition temperature can also been obtained by studying the size dependence of the positions of minima of $V_4(L)$. These values of the pseudocritical temperature were also fitted using a power law as suggested by finite size scaling of the form [8, 9]

$$T = T_\infty(1 - a'L^{-b'}).$$

The best value of T_∞ obtained by our least square subroutine is 0.9955 which is very close to the exact value 0.9949 [1, 2]. The a' and b' obtained is -2.8 and 1.99.

In conclusion we have used the cumulant method in association with the Monte Carlo histogram technique to study the order of phase transition of the two-dimensional Potts model with multispin interaction. Our conclusion is that for $q=3$ the model will change from a second-order transition ($m=2, n=2$) to a first-order transition ($m=3, n=2$).

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