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Interfacial adsorption phenomena of the three-dimensional three-state Potts model

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Abstract. We study the interfacial adsorption phenomena of the three-state ferromagnetic Potts model on the simple cubic lattice by the Monte Carlo method. Finite-size scaling analyses of the net adsorption yield evidence of the phase transition being of first order and $k_B T_C/J = 1.8166(2)$.

1. Introduction

The Potts model is a multi-state statistical mechanical model for spin systems [1–3]. The Potts spin variable takes a value of $1, 2, \ldots,$ and q. The Bragg–Williams approximation predicts that it exhibits a first-order phase transition for $q > 2$ [2].

The properties of the two-dimensional models have been well understood. According to the duality argument, the transition temperature is known for all q exactly [1,2]. Baxter [4] proved the phase transition to be first order for $q > 4$ and second order for $q \leqslant 4$. There is a conjecture for the thermal and magnetic exponents y_t [5] and y_h [6,7] for $q \leqslant 4$.

There is no exact result in three dimensions [3]. There is a problem whether the order of the transition of the three-dimensional three-state Potts model is first order or not. It has been studied by many authors and the result is that it has a weak first-order phase transition [8–18]. The transition is characterized by a small jump in the energy.

The specific heat has a singularity of the delta function type as a result of the discontinuity of the energy at first-order phase transitions. The behaviour can be seen only in systems with infinite lattice size. In systems with finite lattice size the singularity of the energy is smoothed out and that of the specific heat is rounded off. The finite-size scaling theory can predict the behaviour of infinite systems through information about finite systems [19–21].

The Monte Carlo method is a useful tool with which to investigate phase transitions and critical phenomena [22,23]. Monte Carlo simulations are necessarily carried out on systems with finite lattice size. With the help of the finite-size scaling theory we can study the thermodynamic behaviour of various physical systems.

The specific heat of the system with linear size L has a maximum $C_{max}(L)$ at a temperature $T^C_{max}(L)$. The finite-size effects are governed by the dimensions d at first-order phase transitions [24–26]:

$$C_{max}(L) \sim L^d$$

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and

$$T_{\max}^{C}(L) - T_C \sim L^{-d}$$

and by the critical exponents α and ν at second-order transitions [19–21]:

$$C_{\max}(L) \sim L^{\alpha/\nu}$$

and

$$T_{\max}^{C}(L) - T_C \sim L^{-1/\nu}.$$

The difference in power has been used to determine the nature of the transitions [16].

As was described above, the five-state Potts model on the square lattice undergoes a first-order phase transition. Peczak and Landau [27] studied the system using the Monte Carlo method. They found that it behaved as if the transition were second order, i.e. the physical quantities showed pseudocritical behaviour, e.g. $C_{\max}(L) \sim L^{1.09}$ rather than L^2. Thus it is difficult to recognize the order of the transition. Yamagata and Kasono [28], however, found first-order finite-size effects in interfacial adsorption phenomena [29, 30] of the system by the Monte Carlo method.

The aim of this paper is to identify the transition of the three-state ferromagnetic Potts model on the simple cubic lattice and to determine the transition temperature by analysing the finite-size effects in interfacial adsorption phenomena with the Monte Carlo method. The phenomena in three dimensions are studied for the first time. In the next section we describe the interfacial adsorption phenomena and then discuss the finite-size scaling theory for them in section 3. We present the detail of our Monte Carlo simulations in section 4. In section 5 we analyse the Monte Carlo data. A summary is given in section 6.

2. Interfacial adsorption phenomena

Interfacial adsorption phenomena [29, 30] have been observed in the following multi-state models: the Potts models [28, 31–33], the Blume–Capel model [34, 35], and the chiral clock model [36, 37]. We shall explore them for the Potts models.

Let us consider the q-state ferromagnetic Potts model on the $L^{d-1} \times (L+2)$ hypercubic lattice. In the dth direction the fixed boundary conditions are taken and periodic boundary conditions are used in the remaining directions. We fix the Potts spin variables in two states 1 and m, which takes the value of 1 or 2, at the opposite boundaries in the dth direcition, respectively. The Hamiltonian is given by

$$\mathcal{H}_{(1|m)} = -J \sum_{(i,j)} \delta(\sigma_i, \sigma_j) - J \sum_{i}{}' \delta(\sigma_i, 1) - J \sum_{i}{}'' \delta(\sigma_i, m) \tag{1}$$

where δ is Kronecker's delta function, $J(>0)$ is the strength of interactions, the summation for $\langle i, j \rangle$ is over all nearest-neighbour pairs, except those which involve the fixed spins, on the lattice, $\sum_i'$ and $\sum_i''$ denote the summations over lattice sites which adjoin opposite boundaries in the dth direction, respectively.

In the system $\mathcal{H}_{(1|2)}$ at a very low temperature an interface can appear between two phases (called the (1|2) interface). It has been found that the remaining states $3, 4, \ldots,$ and q (called the non-boundary states) are generated in the form of droplets at the interface near

the transition temperature T_C [31, 32]. The interfacial adsorption phenomena are described by the net adsorption defined [31, 32] as

$$W_L \equiv L^{1-d} \sum_i \sum_{n=3}^{q} [\langle \delta(\sigma_i, n) \rangle_{(1|2)} - \langle \delta(\sigma_i, n) \rangle_{(1|1)}] \tag{2}$$

where $\langle \cdots \rangle_{(1|2)}$ and $\langle \cdots \rangle_{(1|1)}$ denote the thermal or Monte Carlo averages for the systems $\mathcal{H}_{(1|2)}$ and $\mathcal{H}_{(1|1)}$, respectively; the summation for i is over all lattice sites except those where the fixed Potts spin variables are located. One should note that the summation for n is over the non-boundary states. The results of Monte Carlo simulations show that $W_L(T)$ has a finite peak near T_C on the finite system [31].

3. Finite-size scaling theory

Yamagata and Kasono [28] have discussed the finite-size effects [32, 33] of the net adsorption. Noting the relation between $W_L(T)$ and the interfacial free energy, they have shown that

$$W_L(T) \approx L\Omega(tL^d) \tag{3}$$

and

$$W_L(T) \approx L^{1-d+y_h}\Omega(tL^{y_t}) \tag{4}$$

at first- and second-order phase transitions, respectively, where Ω is a scaling function, $t = 1 - T/T_C$, and y_t and y_h are the thermal and magnetic exponents, respectively [3, 5–7]. We omit the correction terms for simplicity here. In two dimensions the finite-size scaling (3) and (4) of $W_L(T)$ has been confirmed by the Monte Carlo method [28, 32, 33]. One should note in (3) that $W_L(T_C)$ is proportional to L at first-order phase transitions regardless of the dimensions d.

Yamagata and Kasono [28] have studied the finite-size effects of $W_L(T_C)$ to identify the order of transitions. They found, using the Monte Carlo method, that $W_L(T_C)$ was proportional to L on the two-dimensional five-state Potts model. It is clear evidence that the transition of the system is first order. As was described in section 1, the finite-size effect of the specific heat of the system was not seen to be first order. It is important to choose physical quantities to be analysed.

We shall study the finite-size effects of the net adsorption of the three-dimensional three-state Potts model on the same lines. However, we do not know the value of the transition temperature of the system exactly [3]. We note that $W_L(T)$ has a maximum $W_{max}(L)$ at a temperature $T^W_{max}(L)$ on the system with linear size L. Thus the scaling function $\Omega(x)$ does so. Let x_{max} be a location of the maximum of $\Omega(x)$ [38]. x_{max} satisfies an equation

$$\frac{d\Omega}{dx}(x_{max}) = 0.$$

We consider the case of first-order phase transitions (3) hereafter. Since it is clear that

$$x_{max} = \frac{T_C - T^W_{max}(L)}{T_C} L^d$$

we obtain a relation

$$T^W_{\max}(L) = T_C - T_C x_{\max} L^{-d}. \tag{5}$$

Since $x_{\max}$ is independent of T and L, $W_{\max}(L)$ grows with L:

$$W_{\max}(L) \equiv W_L(T^W_{\max}(L)) \sim L\Omega(x_{\max}). \tag{6}$$

We may expect to estimate the transition temperature and to identify the nature of the transition by analysing the finite-size effects of the net adsorption obtained by the Monte Carlo simulations.

4. Monte Carlo simulations

We use the Metropolis algorithm [22,23] to simulate the systems $\mathcal{H}_{(1|2)}$ and $\mathcal{H}_{(1|1)}$ given by (1) with $q = 3$ on $L^2 \times (L+2)$ simple cubic lattice (L = 10, 12, 14, 16, 18, 20, 24 and 30). The net adsorption is calculated with (2) of $d = q = 3$. We start each simulation from a high temperature with a random configuration and then gradually cool the system. The pseudorandom numbers are generated by the Tausworthe method [39]. Measurements at a temperature are over 10^5 Monte Carlo steps per spin (MCS/spin) after discarding 10^4 MCS/spin to attain equilibrium. Near $T^W_{\max}(L)$ we observe the physical quantities over 10^6 MCS/spin after 5×10^4 MCS/spin for the systems with L = 14, 16, 18, 20, 24 and 30. We have checked that simulations from the ground-state configuration and a random one gave consistent results and there was no hysteresis. We use the coarse-graining scheme to calculate the statistical errors [40]. Each run is divided into ten blocks and the standard deviations are obtained from the ten subaverages.

As was described in the previous section, we want to estimate the maximum of the net adsorption and its position for each lattice size. Since it is difficult to get them from raw Monte Carlo data, we decide to adopt the procedure B-spline smoothing [39]. We fit our Monte Carlo data by the fourth-order B-spline.

5. Monte Carlo results

From now on, for brevity, the physical quantities are presented in units $k_B = 1 = J$.

Figure 1 shows the temperature dependence of the net adsorption $W_L(T)$ defined by (2) with $d = q = 3$ for various lattice sizes. The net adsorption has a finite peak. We plot $W_{\max}(L)$ against L in figure 2. It is clear that $W_{\max}(L)$ is proportional to L. It is consistent with prediction (6) from the finite-size scaling theory. By using linear regression from the data $W_{\max}(L)$ with L = 18, 20, 24 and 30 we obtain a relation: $W_{\max}(L) = 0.092(4) + 0.0382(2)L$. In figure 3, $T^W_{\max}(L)$ is shown for the function of L^{-3}. For systems with large lattice size it agrees well with (5). We estimate T_C to be 1.8166 ± 0.0002 by using linear regression from the data $T^W_{\max}(L)$ with L = 18, 20, 24 and 30; $T^W_{\max}(L) = 1.8166(2) - 41(2)L^{-3}$. The value should be compared with previous results (see table 1).

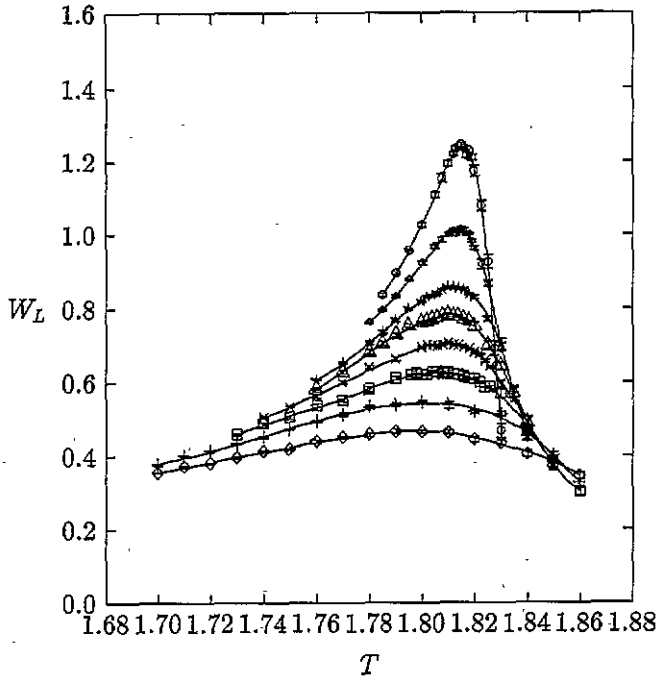

Figure 1. The temperature dependence of the net adsorption of the three-state Potts model on the simple cubic lattice with $L = 10$, 12, 14, 16, 18, 20, 24 and 30. The full curves are obtained by B-spline smoothing. As L increases, the shape of the curve becomes sharper.

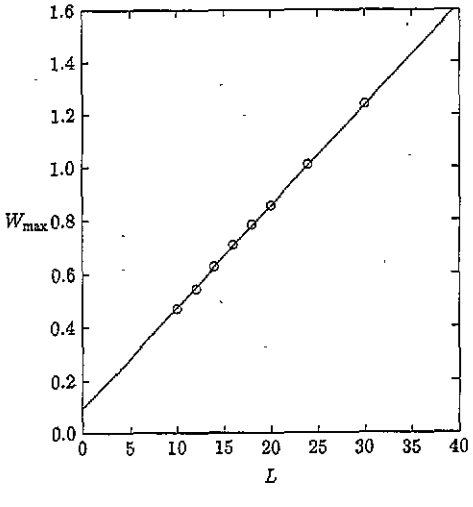

Figure 2. The size dependence of the maximum of the net adsorption of the three-state Potts model on the simple cubic lattice. The full line shows $0.092 + 0.0382L$. Errors are less than symbol size.

6. Summary

We studied the interfacial adsorption phenomena of the three-state ferromagnetic Potts model on a simple cubic lattice. The net adsorption was calculated by the Monte Carlo method. The finite-size effects were consistent with predictions (5) and (6) from the finite-size scaling theory for systems with $L \geqslant 18$. There is clear evidence that the phase transition is first

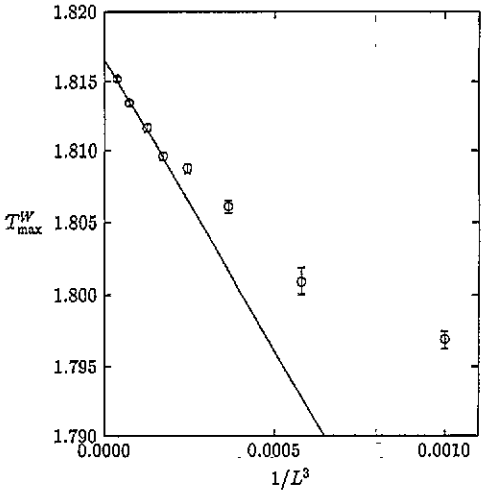

Figure 3. The size dependence of the location of the net adsorption maximum of the three-state Potts model on the simple cubic lattice. The full line shows $1.8166 - 41L^{-3}$.

Table 1. The transition temperature of the three-state Potts model on the simple cubic lattice in units $k_B = 1 = J$.

T_C	Author(s)
1.8166(2)	This work
1.816454(32)	Alves *et al* 1991 [18]
1.8164(1)	Fukugita *et al* 1990 [16]
1.8161(1)	Gavai *et al* 1989 [15]
1.81624(6)	Wilson and Vause 1987 [14]
1.81	Ono and Ito 1982 [13]
1.8169(6)	Knak Jensen and Mouritsen 1979 [12]
1.818(3)	Herrmann 1979 [11]
1.818	Blöte and Swendsen 1979 [10]
1.827(1)	Miyashita *et al* 1979 [9]
1.787(5)	Kim and Joseph 1975 [8]

order. The transition temperature was estimated to be 1.8166(2). It is consistent with recent results [16, 18].

The net adsorption attains to the asymptotic region for $L \geqslant 18$. The specific heat, on the other hand, shows asymptotic behaviour for $L > 30$ [16]. We succeeded in identifying the phase transition and obtaining the transition temperature from the data with $L \leqslant 30$ since we investigated the net adsorption. Generally we can obtain good statistics for small systems on Monte Carlo simulations; however it takes much computer time to simulate large systems. Thus we need to select the observational quantity carefully.

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