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A first-order phase transition in the three-dimensional four-state antiferromagnetic Potts model

Atsushi Yamagata

Department of Physics, Tokyo Institute of Technology, Oh-okayama, Meguro-ku, Tokyo 152, Japan

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Abstract. We study the four-state antiferromagnetic Potts model with next-nearest-neighbour ferromagnetic interactions on the simple cubic lattice by the Monte Carlo method. The ratio J_2/J_1 of the strength of the next-nearest-neighbour interactions to that of the nearest-neighbour interactions is to be 10. We analyse the finite-size effects of the energy, the specific heat, the fourth-order cumulant, the magnetization, the susceptibility and the effective transition temperatures. With the help of the finite-size scaling theory we conclude that the transition of the model is assigned to be of first order.

1. Introduction

At a first-order phase transition, the specific heat and the susceptibility show singularities of the delta function type as a result of discontinuities in the energy and magnetization, respectively. This behaviour can only be seen in the infinite system. Recently much attention has been paid to the effects of the finite size of the system at the transition (Privman 1990). In the finite system, the singularities of the energy and the magnetization are smoothed out and those of the specific heat and the susceptibility rounded off.

Imry (1980) showed for the first time that the finite-size rounding of the transition temperature was proportional to L^{-d} where L was a linear size and d was a spatial dimension of a system.

Binder and Landau (1984) proposed a phenomenological theory for finite-size effects at a field-driven first-order phase transition. The Ising model below the critical temperature undergoes the transition with varying magnetic field. Borgs and Kotecký (1990) discussed the finite-size scaling at the transition from a rigorous point of view.

The q-state ferromagnetic Potts model has a temperature-driven first-order phase transition if q is large enough and $d \geqslant 2$ (Wu 1982). Challa *et al* (1986) studied the finite-size effects at the transition by a phenomenological theory and the Monte Carlo method. Lee and Kosterlitz (1991) studied the transition by a mimic partition function and the Monte Carlo method. Borgs *et al* (1991) discussed the finite-size scaling at the transition from a rigorous point of view.

The results of these studies are that the specific heat and the susceptibility increase with L^d and the effective transition temperature and magnetic field, which are the locations of their extrema, approach the transition temperature and magnetic field

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in the infinite system as L^{-d}, respectively (at the asymmetric field-driven first-order phase transition of the system with the coexistence of two phases, however, as L^{-2d}).

When the previously mentioned discontinuities are small, the transition is called weak. It is well known that the transition of the five-state ferromagnetic Potts model on the square lattice is weak. It is difficult to recognize the order of the transition as first order by numerical methods. Peczak and Landau (1989) analysed the finite-size effect of the specific heat of the model and found that the system behaved as if the transition was second order. Yamagata and Kasono (1992), however, showed that the finite-size effect in the interfacial adsorption phenomena (Selke 1984) of the model was first order even at the weak transition. Although it is useful to investigate finite-size effects to identify the order of the transition (Fukugita *et al* 1990, Lee and Kosterlitz 1990), its success depends on the selection of physical quantities to be analysed.

Researchers have mainly carried out simulations in models with first-order phase transitions: the two-dimensional Ising model in the magnetic field and the Potts models in two dimensions (Baxter 1973). In this paper, for the first time, we study the finite-size effects for a four-state antiferromagnetic Potts model with next-nearest-neighbour ferromagnetic interactions on the simple cubic lattice under fully periodic boundary conditions by the Monte Carlo method. In the next section we describe the model and the results by Banavar and Wu (1984). In section 3 we present definitions of the physical quantities observed in the simulations. We analyse the Monte Carlo data in section 4. In section 5 we discuss the order of the transition on the model.

2. The model

The Hamiltonian of the model studied in this paper is given by

$$\mathcal{H} = J_1 \sum_{(i,j)} \delta(\sigma_i, \sigma_j) - J_2 \sum_{(k,l)} \delta(\sigma_k, \sigma_l) \qquad \sigma_i \in \{1,2,3,4\} \tag{1}$$

where σ_i is a Potts spin variable located at the ith lattice site; δ is Kronecker's delta function; the first summation is over all nearest-neighbour pairs and the second is over all next-nearest-neighbour pairs on a simple cubic lattice; J_1 and J_2 are the strength of the interactions and are both positive.

Banavar and Wu (1984) described a phase diagram of the model using the mean-field approximation. It indicates that when J_2/J_1 is sufficiently large, the model has a first-order phase transition between low-temperature ordered phases and a high-temperature disordered phase. (When J_2/J_1 is small, it undergoes successive phase transitions. A Monte Carlo study for the model in two dimensions was carried out by Grest and Banavar (1981). In this paper they are not discussed.) To understand the ordered phases, let us consider the ground state. It is twelve-fold degenerate because one spin state is favoured on one sublattice, while a different spin state is favoured on the other sublattice, e.g. $\sigma_i = 1$ on the A sublattice and $\sigma_i = 2$ on the B sublattice. They also carried out Monte Carlo simulations on a $12 \times 12 \times 12$ simple cubic lattice. They observed a discontinuity in the order parameter and concluded that the transition was first order.

The singularity, however, can only be seen in the infinite system. It seems that the discontinuity was due to the short Monte Carlo steps which were 1000. There is no hysteresis for the data over many steps even at first-order phase transitions (Challa *et al* 1986).

3. Monte Carlo simulations

We use the Metropolis Monte Carlo technique (Binder 1979) to simulate the model (1) with $J_2/J_1 = 10$ on an $L \times L \times L$ simple cubic lattice under fully periodic boundary conditions. We start each simulation from a high temperature with a random configuration and then gradually cool the system. The pseudo-random numbers are generated by the Tausworthe method (Tsuda 1988). Measurements at a temperature are over 10^6 Monte Carlo steps per spin (MCS/spin) for $L = 6$, 8, 10 and 12, 2×10^6 MCS/spin for $L = 14$ and 3×10^6 MCS/spin for $L = 16$ after discarding 10^5 MCS/spin to attain equilibrium. We have checked that simulations from the ground-state configuration and a random one give consistent results. We use the coarse-graining scheme (Landau 1976) to calculate the statistical errors. Each run is divided into ten blocks and the standard deviations are obtained from the ten subaverages.

We measure the energy per spin

$$E = \langle \mathcal{H} \rangle / L^3 \tag{2}$$

where $\langle \cdots \rangle$ denotes a Monte Carlo average. E/J_1 takes a value $-6J_2/J_1$ when the system with $J_2/J_1 > 0$ is in the ground state described in section 2 and $E/J_1 = 3/4 - (3/2)J_2/J_1$ at infinite temperature. Since $J_2/J_1 = 10$ in our model, $-60 \leqslant E/J_1 \leqslant -14.25$. The specific heat is calculated with

$$C/k_B = \beta^2[\langle \mathcal{H}^2 \rangle - \langle \mathcal{H} \rangle^2]/L^3 \tag{3}$$

where k_B is the Boltzmann constant and $\beta = 1/(k_B T)$. The fourth-order cumulant of the energy (Challa *et al* 1986) is defined by

$$V = 1 - \tfrac{1}{3}\langle \mathcal{H}^4 \rangle / \langle \mathcal{H}^2 \rangle^2. \tag{4}$$

In the infinite system, at a first-order phase transition V takes a non-trivial value $V_{\min} (< \frac{2}{3})$ at the transition temperature and $V = \frac{2}{3}$ at the other temperatures, while for a second-order phase transition $V = \frac{2}{3}$ at all temperatures.

Let us consider a magnetization. For antiferromagnetic models, it is necessary to define sublattice order parameters. According to Ono (1986), in the four-state Potts model, a set of the order parameters is given by

$$\zeta_1^s = (p_1^s + p_2^s - p_3^s - p_4^s)/\sqrt{3}$$
$$\zeta_2^s = (p_1^s - p_2^s - p_3^s + p_4^s)/\sqrt{3}$$
$$\zeta_3^s = (p_1^s - p_2^s + p_3^s - p_4^s)/\sqrt{3}$$
$$p_n^s = 2N_n^s/L^3 \qquad n = 1,2,3,4$$

where s denotes the A or B sublattice and N_n^s is the number of spins which take the value n on the s sublattice. $\langle p_n^s \rangle$ is a probability of a Potts spin having the value n on the s sublattice. p_n^s are satisfied with a condition $\sum_{n=1}^4 p_n^s = 1$ for each sublattice. We measure a quantity, as the magnetization,

$$M = \langle \zeta^- \rangle \tag{5}$$

where $\zeta^- = [\sum_{i=1}^3 (\zeta_i^-)^2]^{1/2}$ and $\zeta_i^- = (\zeta_i^A - \zeta_i^B)/2$. M takes a value $\sqrt{2/3}$ when the system with $J_2/J_1 > 0$ is in the ground state described in section 2 and $M = 0$ at infinite temperature. We define a susceptibility by

$$\chi = L^3[\langle (\zeta^-)^2 \rangle - \langle \zeta^- \rangle^2]. \tag{6}$$

4. Monte Carlo results

As is shown later, we want to estimate extrema of physical quantities for each lattice size, or an intersection between physical quantities with different lattice sizes. Since it is difficult to get them from raw Monte Carlo data, we decided to adopt the procedure of B-spline smoothing (Tsuda 1988). We fitted our Monte Carlo data by the fourth-order B-spline.

Hereafter, for brevity, the physical quantities are presented in units $k_B = 1 = J_1$.

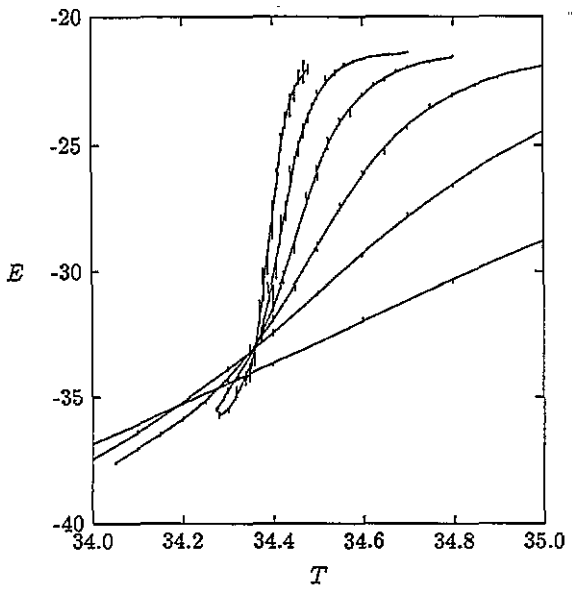

Figure 1. The temperature dependence of the energy per spin for $L = 6$, 8, 10, 12, 14 and 16. The vertical lines denote Monte Carlo data with error bars. The full curves are obtained by the B-spline fitting. As L increases, the slope of the curve becomes steeper.

4.1. Energy

Figure 1 shows the temperature dependence of the energy per spin $E(T, L)$ defined by (2) for various lattice sizes. There is an intersection between the curves with different size L. Let us define an effective transition temperature $T^E_{\rm cross}(L)$ in a finite system by $E(T^E_{\rm cross}(L), L) = E(T^E_{\rm cross}(L), L+2)$ (Borgs *et al* 1991, Borgs and Janke 1992). In figure 2 the size dependence of $T^E_{\rm cross}(L)$ is presented. It does not exhibit monotonic behaviour and there is a maximum. It is difficult to extrapolate T_C which is the transition temperature in the infinite system because of this behaviour. As a function of L, $E(T^E_{\rm cross}(L), L)$ behaves like $T^E_{\rm cross}(L)$.

4.2. Specific heat

Figure 3 shows the temperature dependence of the specific heat $C(T, L)$ defined by (3) for various lattice sizes. We plot the specific heat maximum $C_{\rm max}(L)$ against L^3

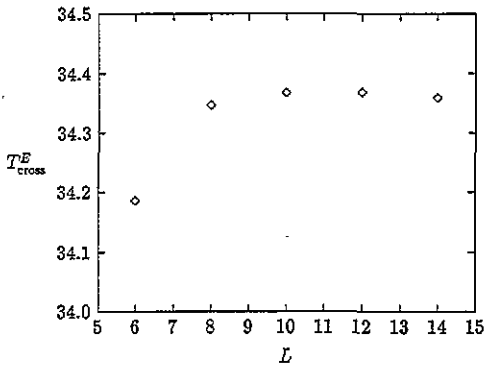

Figure 2. The size dependence of the effective transition temperature defined by $E(T^E_{cross}(L), L) = E(T^E_{cross}(L), L+2)$. Errors are less than symbol size.

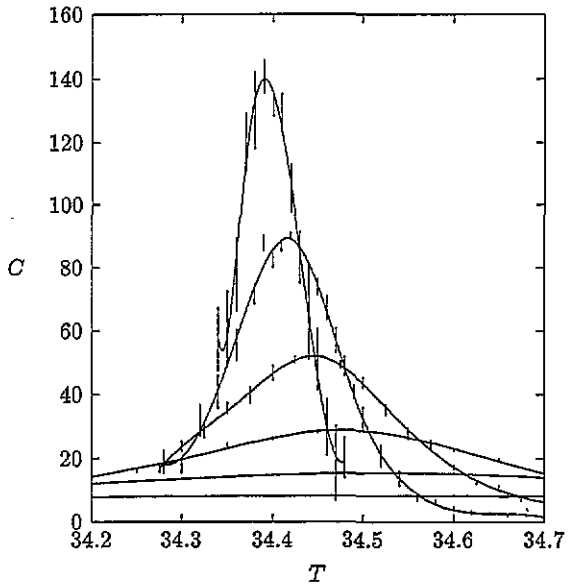

Figure 3. The temperature dependence of the specific heat. The meaning of the curves and the vertical lines is the same as in figure 1. As L increases, the shape of the curve becomes sharper.

in figure 4. It is clear that $C_{max}(L)$ is proportional to L^3 for large L:

$$C_{max}(L) = a_0 + a_1 L^3 \tag{7}$$

where a_0 and a_1 are constants. In figure 5 the location $T^C_{max}(L)$ of $C_{max}(L)$ is plotted against L^{-3}. Although the approach to the asymptotic behaviour seems to be slow, it is consistent with a prediction of the finite-size scaling theory at a first-order phase transition:

$$T^C_{max}(L) = T_C + a_2 L^{-3} \tag{8}$$

where a_2 is a constant. We obtain a result $T_C = 34.354 \pm 0.009$ by using the linear regression from the data $T^C_{max}(L)$ with $L = 12$, 14 and 16.

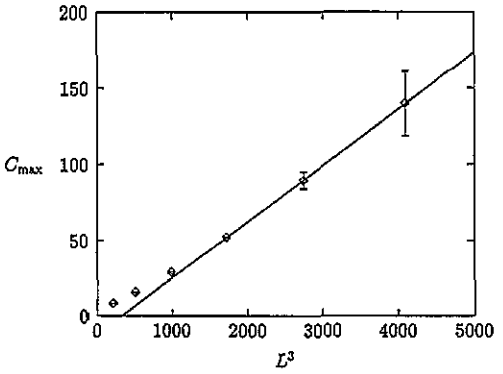

Figure 4. The size dependence of the specific heat maximum. The full line obtained by the linear regression shows $-12.2(6) + 0.0371(2)L^3$.

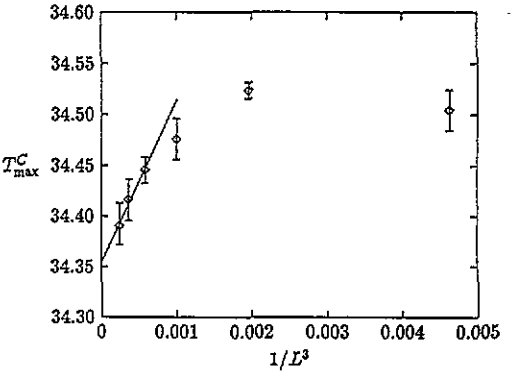

Figure 5. The size dependence of the effective transition temperature defined as the location where the specific heat takes the maximum. The full line obtained by the linear regression shows $34.354(9) + 160(21)L^{-3}$.

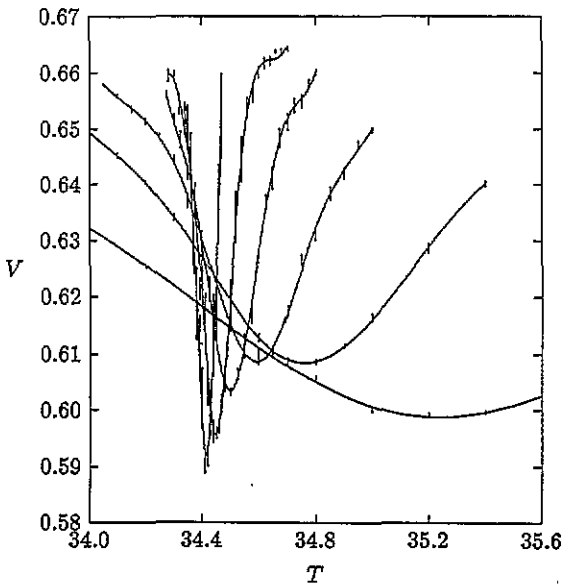

Figure 6. The temperature dependence of the fourth-order cumulant of the energy. The meaning of the curves and the vertical lines is the same as in figure 1. As L increases, the shape of the curve becomes sharper.

4.3. Fourth-order cumulant

Figure 6 shows the temperature dependence of the fourth-order cumulant $V(T, L)$ of the energy defined by (4) for various lattice sizes. In figure 7 the size dependence of the fourth-order cumulant minimum $V_{min}(L)$ is shown against L^{-3}. For large L, the approach to V_{min} which is the value of the infinite system may be approximate to the relation: $V_{min}(L) = V_{min} + b_1 L^{-3}$ where b_1 is a positive constant. It is a result of the finite-size scaling theory at a first-order phase transition. By using the linear-

regression from the data $V_{min}(L)$ with $L = 12$, 14 and 16, we estimate V_{min} to be 0.5836 ± 0.0008. An effective transition temperature $T^V_{min}(L)$ which is the location of $V_{min}(L)$ is plotted against L^{-3} in figure 8. The behaviour is consistent with a result of finite-size scaling theory: $T^V_{min}(L) = T_C + b_2 L^{-3}$ with a positive constant b_2. From the data $T^V_{min}(L)$ with $L = 12$, 14 and 16, we obtain a result $T_C = 34.355 \pm 0.003$.

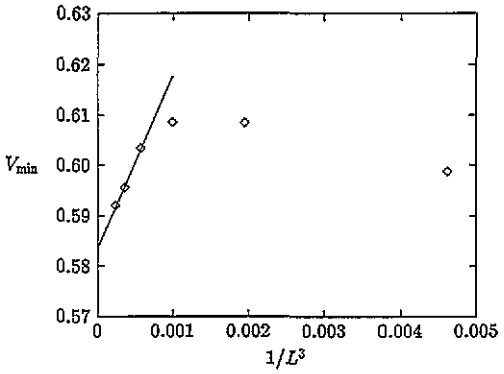

Figure 7. The size dependence of the minimum of the fourth-order cumulant of the energy. The full line obtained by the linear regression shows $0.5836(8) + 34(2)L^{-3}$. Errors are less than symbol size.

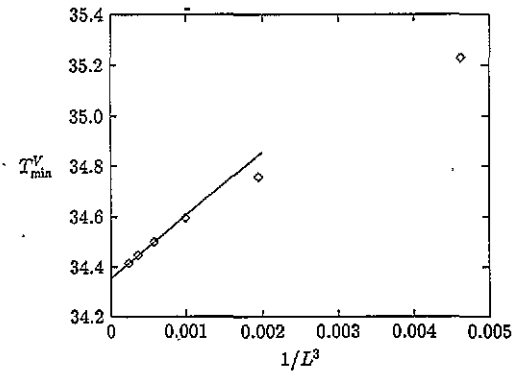

Figure 8. The size dependence of the effective transition temperature defined as the location where the fourth-order cumulant takes the minimum. The full line obtained by the linear regression shows $34.355(3) + 251(7)L^{-3}$. Errors are less than symbol size.

We will give an another effective transition temperature in a finite system. Let us consider $V(T, L)$ of the system with the lattice size L below $T^V_{min}(L)$ in figure 6. We see that there is an intersection between the curves with L and $L + 2$ ($L = 8$, 10, 12 and 14) and the position may tend to T_C which is estimated from $C(T, L)$ or $\chi(T, L)$. Thus we define $T^V_{cross}(L)$ by

$$V(T^V_{cross}(L), L) = V(T^V_{cross}(L), L + 2) \tag{9}$$

and show it in figure 9. T_C is estimated to be 34.341 by the least-squares fitting assuming

$$T^V_{cross}(L) = T_C + b_3 \exp(-L/L^V_{cross}) \tag{10}$$

where T_C, b_3 and L^V_{cross} are the parameters of the fitting.

4.4. Magnetization

Figure 10 shows the temperature dependence of the magnetization $M(T, L)$ defined by (5) for various lattice sizes. The behaviour is similar to that of $-E(T, L)$ as is shown in figure 1. By analogy with $T^E_{cross}(L)$, we define an effective transition temperature $T^M_{cross}(L)$ as follows

$$M(T^M_{cross}(L), L) = M(T^M_{cross}(L), L + 2). \tag{11}$$

Figure 11 shows the size dependence of $T^M_{cross}(L)$ as a function of L. Assuming

$$T^M_{cross}(L) = T_C + c \exp(-L/L^M_{cross}) \tag{12}$$

where T_C, c and L^M_{cross} are the parameters of the fitting, we obtain results $T_C = 34.355$ and 34.359 for $L = 6$–14 and 8–14, respectively. We observe that the value of $M(T^M_{cross}(L), L)$ decreases rapidly as L increases and then may saturate.

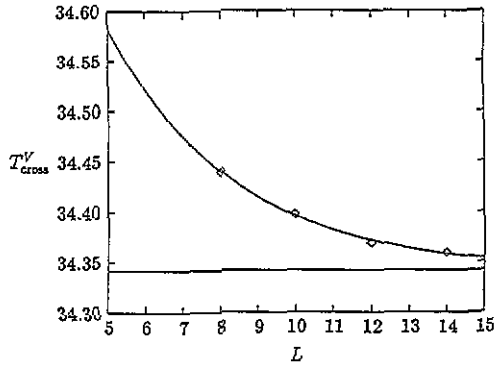

Figure 9. The size dependence of the effective transition temperature defined by (9). The full curve obtained by the least-squares fitting shows $34.341 + 1.07\exp(-L/3.35)$. The horizontal line denotes $T = 34.341$. Errors are less than symbol size.

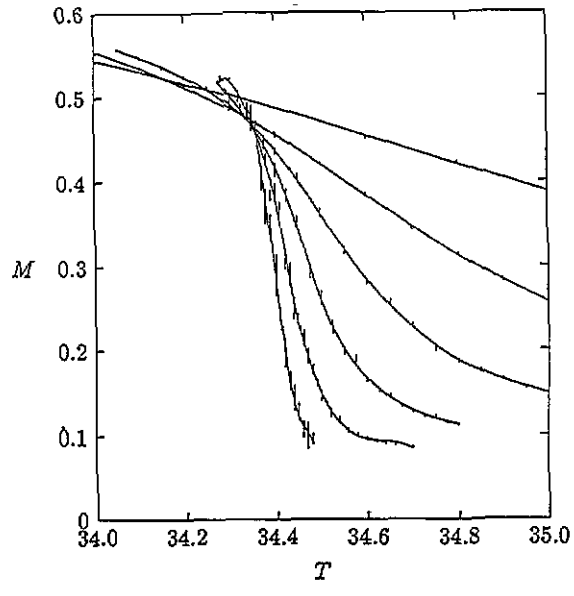

Figure 10. The temperature dependence of the magnetization. The meaning of the curves and the vertical lines is the same as in figure 1. As L increases, the slope of the curve becomes steeper.

4.5. Susceptibility

The behaviour of the susceptibility $\chi(T, L)$ defined by (6) is similar to that of $C(T, L)$ as is shown in figure 3. The susceptibility maximum $\chi_{max}(L)$ is proportional to L^3 as is shown in figure 4 and behaves as $\chi_{max}(L) = -31(2) + 0.0489(6)L^3$ for $L = 12$, 14 and 16. An effective transition temperature $T^{\chi}_{max}(L)$ which is the location of $\chi_{max}(L)$ approaches T_C similar to $T^{\chi}_{max}(L)$ as is shown in figure 8 and behaves as $T^{\chi}_{min}(L) = 34.344(5) + 208(12)L^{-3}$ for $L = 12$, 14 and 16.

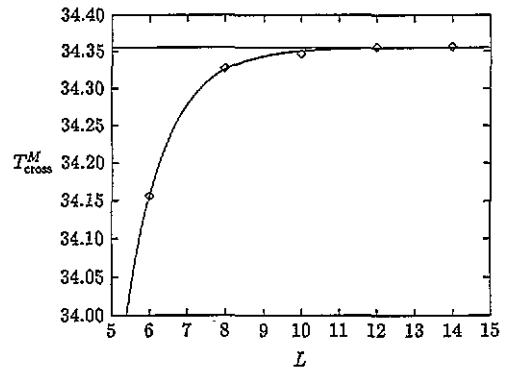

Figure 11. The size dependence of the effective transition temperature defined by (11). The full curve obtained by the least-squares fitting shows $34.355 - 60.8\exp(-L/1.05)$. If we neglect the data of $L = 6$, then we get the result $34.359 - 1.78\exp(-L/2.00)$. The horizontal line denotes $T = 34.355$. Errors are less than symbol size.

5. Discussions

By the Monte Carlo method we have calculated the energies, the specific heats, the fourth-order cumulants, the magnetizations and the susceptibilities of the four-state antiferromagnetic Potts model which includes next-nearest-neighbour ferromagnetic interactions ($J_2 = 10$) on the simple cubic lattices.

There were intersections between the curves of $E(T, L)$ with L and $L + 2$. The existence of the intersections on the q-state Potts models was proved for $d \geqslant 2$ and q large enough (Borgs *et al* 1991, Borgs and Janke 1992) and was founded for $d = 3$ and $q = 3$ by the Monte Carlo simulations (Fukugita *et al* 1990). It may be characteristic of temperature-driven first-order phase transitions. According to the finite-size scaling theory, one has a relation $|T^E_{cross}(L) - T_C| = O(e^{-\text{constant}\cdot L})$. Although we could not confirm it, we observed $T^E_{cross}(L)$ tended to T_C rapidly.

$C_{max}(L)$ and $\chi_{max}(L)$ grew with L^3 and $T^C_{max}(L)$ and $T^\chi_{max}(L)$ approached T_C from above as L^{-3} for large L. The results are consistent with the predictions of the finite-size scaling at first-order phase transitions.

It is well known that the fourth-order cumulant of the energy plays a role as an indicator to identify the nature of transitions (Challa *et al* 1986). $V_{min}(L)$ and $T^V_{min}(L)$ of our model showed the characteristic behaviour of first-order phase transitions.

On account of these results we conclude that the transition of the model (1) with $J_2 = 10$ is first order. We think that our model has a transition with the coexistence of twelve ordered phases and one disordered phase at the transition temperature.

We defined the new effective transition temperatures by (9) and (11) and found that they behaved as (10) and (12), respectively. The values T_C extrapolated from $T^M_{cross}(L)$ and $T^V_{cross}(L)$ agreed with those from $T^C_{max}(L)$, $T^V_{min}(L)$ and $T^\chi_{max}(L)$ within errors. Therefore it seems that our definitions are reasonable.

At last we will mention the latent heat l which is the energy gap at the transition temperature in the infinite system. According to the finite-size scaling theory (Lee and Kosterlitz 1991), a_1 in (7) and a_2 in (8) are related to l as follows: $a_1 = \frac{1}{4}l^2/T_C^2$ and $a_2 = l^{-1}T_C^2 \ln q$ where q is the number of the low-temperature phases. They are clearly positive numbers. We can estimate l from the slopes in figures 4 and 5 using

$T_C = 34.354 \pm 0.009$ and $q = 12$. Unfortunately we did not get consistent results: $l = 13.23 \pm 0.04$ and 18 ± 2, respectively.

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