Finite-size effects of dimensional crossover in quasi-two-dimensional three-state Potts model

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Abstract
A nearest neighbour spin pair of the quasi-two-dimensional three-state Potts model interacts with the strength $J (> 0)$ in the $xy$-plane and with $\lambda J$ ($0 \leq \lambda \ll 1$) in the $z$-axis. The phase transition is of second-order when $\lambda = 0$ and is of first-order when $\lambda > 0$. The dimensional crossover occurs with a change of the order of the phase transition. We study the finite-size effects of the phenomenon by using a Monte Carlo method with a multi-spin coding technique. The prediction of the finite-size scaling theory is consistent with the Monte Carlo results.
1 Introduction

A quasi-two-dimensional system is a three-dimensional one in which the ratio $\lambda$ of the interplanar to the intraplanar exchange interactions is small. If the system exhibits a phase transition, we can see a crossover from two-dimensional to three-dimensional behaviour as the critical point is approached. Many authors have studied quasi-two-dimensional antiferromagnets by neutron scattering experiments [1]. The theoretical studies of the dimensional crossover have been carried out by using perturbation theory [2]-[5], high temperature series expansion [6]-[13], generalized homogeneous functions [14], and rigorous approach [15]-[17]. The results are that the critical and the crossover temperature are singular with respect to $\lambda$. They behave as $\lambda^{1/\phi}$ where $\phi$ is the crossover exponent [18]. It has been shown that $\phi$ is equal to the critical exponent $\gamma$ for the susceptibility of the system with $\lambda = 0$. The present author discussed finite-size scaling and performed Monte Carlo simulations of the quasi-two-dimensional Ising model for the first time [19].

In the above mentioned researches there was an assumption that the order of the phase transition was unaltered. In this paper we study finite-size scaling of the dimensional crossover in which it changes. We perform Monte Carlo simulations of the three-state ferromagnetic Potts model [20]. The phase transition is of second-order in two dimensions [21] and is of first-order in three dimensions [22]. In the next section we review the finite-size scaling theory for the quasi-two-dimensional systems briefly. The finite-size scaling form of an effective transition temperature is presented. In section 3 we describe an algorithm for the multi-spin coding technique used in our Monte Carlo simulations of the quasi-two-dimensional three-state Potts model. The Monte Carlo data are compared with the prediction of the finite-size scaling theory in section 4. A summary is given in section 5.

2 Finite-size scaling theory

We review the finite-size scaling theory for the quasi-two-dimensional systems briefly. The detailed discussion is in the reference [19]. Let us consider the three-state Potts model on the simple cubic lattice for the sake of con-
creteness. The Hamiltonian is

$$\mathcal{H}_\lambda = \sum_{\langle ij \rangle} J_{ij} [1 - \delta(\sigma_i, \sigma_j)] + H \sum_i [1 - \delta(\sigma_i, 1)]$$

(1)

where $\sigma_i$ is a Potts spin variable located $i$th lattice site and which takes on the value 1, 2, and 3. The first summation is over all nearest neighbour pairs on the lattice, the second summation over all lattice sites. The strength $J_{ij}$ of the interaction for the nearest neighbour pair $ij$ is $J(>0)$ in the $xy$-plane and $\lambda J$ ($0 \leq \lambda \ll 1$) in the $z$-axis. $H$ is an external magnetic field. When $\lambda = 0$, the equation (1) consists of two-dimensional three-state ferromagnetic Potts models which are independent of each other.

We assume that the free energy per spin measured by $k_B T$, where $k_B$ is Boltzmann’s constant and $T$ is the temperature, is a generalized homogeneous function of variables $t_0 = T/T(0) - 1$, $h = H/k_B T$, and $\lambda$ as $t_0$, $h$, $\lambda \to 0$, where $T(0)$ is the critical temperature of the system with $\lambda = 0$. We can derive

$$f(t_0, h, \lambda) = |t_0|^{2-\alpha} f^\pm(h/|t_0|^{\beta+\gamma}, \lambda/|t_0|^{\phi})$$

(2)

with a scaling function $f^\pm(x,y)$ where $+$ ($-$) refers to $t_0 > 0$ ($t_0 < 0$), and $\alpha + 2\beta + \gamma = 2$ where $\alpha$, $\beta$, and $\gamma$ are the critical exponents of the two-dimensional system for the specific heat, the magnetization, and the susceptibility, respectively. The number $\phi$ is the crossover exponent and is equal to $\gamma$. From (2) we get the behaviour of $T(\lambda)$ that is the transition temperature of the system with $\lambda$ as follows.

$$T(\lambda)/T(0) - 1 = A^T \lambda^{1/\phi}$$

(3)

where $A^T$ is a constant.

Let us consider the three-state Potts model (1) on an $L \times L \times L$ simple cubic lattice to see the finite-size effects [23]-[25] of (3). To avoid surface effects we impose periodic boundary conditions. We assume that the free energy per spin is a generalized homogeneous function of $t_0$, $h$, $\lambda$, and $L$ as $t_0$, $h$, $\lambda$, $1/L \to 0$ and the system is characterized by $L/\xi(t_0)$ where $\xi(t_0)$ is
the correlation length of the system of \( h = \lambda = 1/L = 0 \). Using (2) we can derive
\[
\tilde{f}(t_0, h, \lambda, L) = L^{-(2-\alpha)/\nu} \tilde{f}(t_0 L^{1/\nu}, h L^{(\beta+\gamma)/\nu}, \lambda L^{\phi/\nu})
\]
where \( \tilde{f}(x, y, z) \) is a scaling function and \( \nu \) is the critical exponent for \( \xi(t_0) \).

Let us define an effective transition temperature as the position, \( T_L(\lambda) \), of the peak of the specific heat. From (4) we get
\[
T_L(\lambda)/T(0) - 1 = L^{-1/\nu} \tilde{T}(\lambda L^{\phi/\nu})
\]
where \( \tilde{T}(x) \) is a scaling function. If \( \tilde{T}(x) \rightarrow A T x^{1/\phi} \) as \( x \rightarrow +\infty \), the equation (3) is reproduced in the limit \( L \rightarrow +\infty \) for a fixed value of \( \lambda(>0) \).

The prediction (5) will be compared with the Monte Carlo data in section 4.

3 Monte Carlo simulations

To confirm the prediction (4) of the finite-size scaling theory, we perform Monte Carlo simulations \([26, 27]\) of the quasi-two-dimensional three-state Potts model \([1]\) in \( H = 0 \) on the \( L \times L \times L \) simple cubic lattice under fully periodic boundary conditions. We use a multi-spin coding technique \([28, 29]\) to simulate a large number of systems simultaneously. Since the FORTRAN compiler on the HITAC S-820/80 computer, we have used, treats 32-bit integers, we can update 32 systems independently. Three-state Potts spin variables located at identical lattice sites are stored in the 32-bit positions of two words \([30, 31]\).

An algorithm is as follows. Let us consider a flip of a spin \( \sigma_0 \). The change in the energy on flipping the spin, \( \sigma_0 \rightarrow \sigma'_0 \), is
\[
\Delta E/J = -\sum_{j=1}^{4} \{[1 - \delta(\sigma_0, \sigma_j)] - [1 - \delta(\sigma'_0, \sigma_j)]\} - \lambda \sum_{k=5}^{6} \{[1 - \delta(\sigma_0, \sigma_k)] - [1 - \delta(\sigma'_0, \sigma_k)]\}
\]
where \( \sigma_j (j = 1, 2, 3, 4) \) is the nearest neighbour spin of \( \sigma_0 \) in the \( xy \)-plane and \( \sigma_k (k = 5, 6) \) in the \( z \)-axis. Using variables
\[
n_{xy} = \sum_{j=1}^{4} \{[1 - \delta(\sigma_0, \sigma_j)] - [1 - \delta(\sigma'_0, \sigma_j)] + 1\}
\]
and

\[ n_z \equiv \sum_{k=5}^{6} \{ [1 - \delta(\sigma_0, \sigma_k)] - [1 - \delta'(\sigma_0, \sigma_k)] + 1 \}, \]

we have

\[ -\Delta E/J = n_{xy} + \lambda n_z - 4 - 2\lambda. \]

Defining a variable \( n \equiv 5n_{xy} + n_z + 10 \), we may see the energy change as a function of \( n \): \((-\Delta E/J)_n, n \in \{10, 11, \ldots, 54\} \).

Using a random variable \( W \) which takes an integer value, we flip the spin if \( n + w \geq 32 \) where \( w \) is a possible value of \( W \). The distribution of \( W \) is determined by

\[
\text{Prob}\{W \geq 32 - n\} = \min(e^{K(-\Delta E/J)_n}, 1) = \begin{cases} e^{K(-\Delta E/J)_n}, & 10 \leq n < 32, \\ 1, & 32 \leq n \leq 54, \end{cases}
\]

where \( K = J/k_B T \). Thus the update is accepted with the probability \( \min(e^{-\beta \Delta E}, 1) \) where \( \beta = 1/k_B T \). This is the same procedure as of the Metropolis algorithm \[32\]. We express \( n + w \ (\in \{10, 11, \ldots, 76\}\) which can be calculated with logical operations, as the binary notation: \( \sum_{l=0}^{6} x_l2^l \), \( x_l \in \{0, 1\} \). In our algorithm we carry out the update when \( x_5 = 1 \) or \( x_6 = 1 \) although the Metropolis procedure needs to refer to the inequality \( r \leq \min(e^{-\beta \Delta E}, 1) \) where \( r \) is a possible value of a random variable \( R \) with uniform distribution over \([0,1]\). The algorithm explained here is for \( \lambda \in (0, 1/4) \). It is sufficient to study the system since we are interested in the case of the small value of \( \lambda \).

The pseudorandom numbers are generated by the Tausworthe method \[33, 34\]. We measure physical quantities at a temperature over \(10^5 \) Monte Carlo steps per spin (MCS/spin) after discarding \(10^4 \) MCS/spin to attain equilibrium. Physical quantities are calculated by the multi-step bitwise summation algorithm \[33, 34\]. Our algorithm achieves a speed of 25 million spins per second on a \(30 \times 30 \times 30\) lattice with measurements at every step. Let us denote the average of a physical quantity, \( O \), in each system by \( \langle O \rangle_i, i = 1, 2, \ldots, 32 \). The expectation value is given by

\[
\langle O \rangle = \frac{1}{32} \sum_{i=1}^{32} \langle O \rangle_i,
\]
the standard deviation by
\[ \Delta\langle O \rangle = \left( \langle O \rangle^2 - \langle O \rangle^2 \right)^{1/2} / \sqrt{31}. \]

4 Monte Carlo results

In the reference [19] we reported that there was hysteresis in magnetic quantities (magnetization, susceptibility, . . . ) but we could not see it in the energy, the specific heat:
\[ C = k_B \beta^2 \left( \langle H^2 \rangle - \langle H \rangle^2 \right) / L^3, \]
and the fourth-order cumulant of the energy for the small value of \( \lambda \) or a small number of MCS/spin. The hysteresis vanished for the large value of \( \lambda \) or a large number of MCS/spin. We have observed similar behaviour for the quasi-two-dimensional three-state Potts model. According to [19], we analyse the peak position, \( T_L(\lambda) \), of the specific heat since we can obtain useful information about phase transitions from it.

Figure 1 shows the temperature dependence of \( C \) of \( L = 20 \) system for various \( \lambda \). The solid curves are obtained by the smoothing procedure of the fourth-order B-spline [33]. As \( \lambda \) increases, the shape of the curve becomes sharper and the peak position \( T_{20}(\lambda) \) becomes higher. Then we get the peak height and \( T_{20}(\lambda) \).

Figure 2 shows the finite-size scaling plot of \( T_L(\lambda) \). We have used the exact values of the critical temperature, \( k_B T(0)/J = 1/\ln(1 + \sqrt{3}) \), and the critical exponents, \( \phi = \gamma = 13/9 \) and \( \nu = 5/6 \), of the two-dimensional three-state ferromagnetic Potts model [20]. The data fall on a common curve. It is consistent with (5). The slope seems to approach \( 1/\phi = 1/\gamma = 9/13 \). It indicates that the asymptotic behaviour of the finite-size scaling function is \( \tilde{T}(x) \to \text{const.} \times x^{1/\phi} \) as \( x \to +\infty \).

5 Summary

The dimensional crossover occurs with a change of the order of the phase transition in the quasi-two-dimensional three-state Potts model. We have studied the finite-size effects of the phenomenon by using a Monte Carlo method. An algorithm of a multi-spin coding technique for this model has
been presented. The prediction (5) of the finite-size scaling theory has been consistent with the Monte Carlo results. We have seen the asymptotic behaviour of the finite-size scaling function on the system with $\lambda \leq 0.24$ and $L \leq 30$.

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Figure captions

**Figure 1** Temperature \((K = J/k_BT)\) dependence of the specific heat of the \(L = 20\) system for various \(\lambda\): 0.04, 0.08, 0.1, 0.12, 0.14, 0.16, 0.18, 0.20, 0.22, 0.24. The solid curves are obtained by the smoothing procedure of the fourth-order \(B\)-spline. As \(\lambda\) increases, the shape of the curve is sharper and \(T_{20}(\lambda)\) becomes higher.

**Figure 2** Finite-size scaling plot of the effective transition temperature. The data of the system with \(L = 10, 20,\) and 30 are denoted by \(\bigcirc, \times,\) and \(\Box\), respectively. We have set that \(k_BT(0)/J = 1/\ln(1+\sqrt{3})\), \(\phi = \gamma = 13/9,\) and \(\nu = 5/6\). The data fall on a common curve. The solid line shows that \((9/13) \ln(\lambda L^{26/15})\). Errors are less than the symbol size.
Figure 1
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\[ \ln\left\{ \frac{T_L(\lambda)}{T(0)} - 1 \right\} L^{1/\nu} \]

**Figure 2**

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