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2001 J. Phys. A: Math. Gen. 34 8781

(http://iopscience.iop.org/0305-4470/34/42/305)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND GENERAL

J. Phys. A: Math. Gen. **34** (2001) 8781–8794 PII: S0305-4470(01)25320-7

Three-dimensional antiferromagnetic q-state Potts models: application of the Wang–Landau algorithm

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Received 22 May 2001, in final form 28 August 2001
Published 12 October 2001
Online at stacks.iop.org/JPhysA/34/8781

Abstract

We apply a newly proposed Monte Carlo method, the Wang–Landau algorithm, to the study of the three-dimensional antiferromagnetic q-state Potts models on a simple cubic lattice. We systematically study the phase transition of the models with $q = 3$, 4, 5 and 6. We obtain the finite-temperature phase transition for $q = 3$ and 4, whereas the transition temperature is down to zero for $q = 5$. For $q = 6$ there exists no order for any temperature. We also study the ground-state properties. The size dependence of the ground-state entropy is investigated. We find that the ground-state entropy is larger than the contribution from the typical configurations of the broken-sublattice-symmetry state for $q = 3$. The same situations are found for $q = 4$, 5 and 6.

PACS numbers: 75.10.Hk, 05.10.Ln, 05.50.+q

1. Introduction

The q-state Potts model has various interesting properties to study [1–3]. The order of the phase transition of the Potts model depends on the spatial dimensionality and the number of states, q. The phase transitions of the antiferromagnetic (AF) Potts models are more complex than those of the ferromagnetic Potts models. Here, we focus on the three-dimensional AF q-state Potts models. Banavar *et al* [4] studied the AF three- and four-state Potts models by use of the Monte Carlo simulation. Ono [5] pointed out an appropriate choice of the vector order parameter for the AF Potts models on a bipartite lattice. The phase transition of the AF three-state Potts model is considered to belong to the XY universality class [6, 7]. The low-temperature phase of the AF three-state Potts model was shown to be the broken-sublattice-symmetry (BSS) state, but it is still an open question whether a rotationally symmetric state exists or not below the second-order phase transition point of the XY universality class [8–11]. Compared with the AF three-state Potts model, there not have been so many systematic studies on the AF four-state and higher-state Potts models in three dimensions. Recently, the AF four-state Potts model was studied by Itakura [12]; there is a finite-temperature phase transition, and

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the critical phenomena may belong to the Heisenberg universality class if the phase transition is of second order. However, the possibility of a first-order transition was also argued [12]. Another source of interest in AF q-state Potts models is that they have nonzero ground-state entropy without frustration. Nonzero ground-state entropy, $S_0 \neq 0$, is an important subject in statistical mechanics. One physical example is provided by ice. The AF Potts model serves as a useful model for the study of the nonzero ground-state entropy, and the nonzero ground-state entropy of the two-dimensional AF Potts model was extensively studied by Shrock and Tsai [13].

Monte Carlo simulation is regarded as a standard tool for studying statistical mechanical properties [14]. The Monte Carlo study using a conventional Metropolis algorithm sometimes suffers from the problem of slow dynamics, or the long-timescale problem. In the study of the phase transition, the long timescale due to the critical slowing-down causes the problem of slow equilibration. For the simulational study of the AF Potts models, the cluster algorithm [15] has been used [6, 7, 9, 10, 12] to overcome the critical slowing-down. As an extension of the cluster algorithm, Tomita and Okabe [16] recently proposed a new cluster algorithm of tuning the critical point automatically, and applied it to the study of 2D Potts models. The extended ensemble method is another type of attempt to overcome the slow dynamics. The multicanonical method [17, 18], simulated tempering [19], the exchange Monte Carlo method [20] (or the multiple-Markov-chain method [21]), the broad-histogram method [22] and the flat-histogram method [23] are examples of the extended ensemble method. Quite recently, Wang and Landau [24] proposed an efficient algorithm to calculate the density of states with high accuracy. In the present paper we use the Wang–Landau algorithm [24] to study the three-dimensional AF Potts models. We study not only the phase transition of the AF Potts models but also the ground-state properties. The Wang–Landau algorithm is quite effective for this purpose because we can calculate the density of states with high accuracy. We make a random walk in the whole energy space, and the algorithm is appropriate for calculating the ground-state entropy.

We organize the rest of the paper as follows. In section 2, we describe the model and the vector order parameter for the AF Potts model. We also briefly explain the simulation method, the Wang–Landau algorithm. In section 3, we study the phase transition of the AF three-, four-, five- and six-state Potts models on a simple cubic lattice. The ground-state properties of the three-, four-, five- and six-state Potts models are studied in section 4. The summary and discussions are given in section 5.

2. Model and simulation method

We deal with the AF Potts model defined by the Hamiltonian

$$\mathcal{H} = J \sum_{\langle i,j \rangle} \delta_{\sigma_i,\sigma_j} \qquad (J > 0) \tag{1}$$

where the Potts variable σ_i takes the value $1, 2, \ldots, q$, and the summation is taken over the nearest-neighbour pairs of sites on a simple cubic lattice.

The ferromagnetic three-state Potts model can be transformed into the Z_3 clock model, and the order parameter is well represented by a two-dimensional vector. For the AF Potts model on a bipartite lattice, the sublattice structure should be taken into account [5, 25]; that is, the staggered magnetization will be treated. Using three components of the staggered magnetization

$$m_i = \frac{1}{N}\left(\sum_{j \in \mathrm{A}} \delta_{\sigma_j,i} - \sum_{j \in \mathrm{B}} \delta_{\sigma_j,i} \right) \tag{2}$$

where A and B denote two sublattices, we define the vector order parameter as follows:

$$\boldsymbol{M} \equiv m_1\boldsymbol{e}_1 + m_2\boldsymbol{e}_2 + m_3\boldsymbol{e}_3. \tag{3}$$

Here, $\boldsymbol{e}_i$ denotes the unit vectors in two dimensions directed 120° apart from each other, and

$$\boldsymbol{e}_1 + \boldsymbol{e}_2 + \boldsymbol{e}_3 = 0. \tag{4}$$

Then, the square of the vector order parameter simply becomes

$$M^2 = \tfrac{3}{2}\left(m_1^2 + m_2^2 + m_3^2\right). \tag{5}$$

We can extend the above argument to higher-state Potts models [5]. In general the order parameter of the q-state Potts model is well described by the $(q-1)$-dimensional vector order parameter. We consider the unit vectors in $(q-1)$ dimensions pointing to q directions as in the case of the three-state Potts model; the sum of the unit vectors is set to be zero as in equation (4). Using each component of the staggered magnetization, equation (2), we can obtain the generalized expression for equation (5)

$$M^2 = \frac{q}{q-1}\left(m_1^2 + m_2^2 + \cdots + m_q^2\right). \tag{6}$$

We should note that for the three-state Potts model the vector order parameter space spans a hexagonal region in a two-dimensional space, and the maximum value of $|\boldsymbol{M}|$ is $\sqrt{3}/2$. For the four-state Potts model the order parameter takes the values within the area shown in figure 3 of [12], and the maximum value of $|\boldsymbol{M}|$ is $\sqrt{2/3}$.

We briefly describe the Wang–Landau algorithm [24]. This algorithm is similar to Lee's version of the multicanonical method (entropic sampling) [18], the broad-histogram method [22] and the flat-histogram method [23]; but the Wang–Landau algorithm has advantage that it can estimate the density of states efficiently even for large systems. The idea of the Wang–Landau algorithm [24] is that we make a random walk in energy space based on the transition probability from energy level E_1 to E_2

$$p(E_1 \to E_2) = \min\left[\frac{g(E_1)}{g(E_2)}, 1\right] \tag{7}$$

where $g(E)$ is the density of states. Since the exact form of $g(E)$ is not known *a priori*, we determine $g(E)$ iteratively; $g(E)$ is modified by

$$\ln g(E) \to \ln g(E) + \ln f_i \tag{8}$$

every time the state is visited. The modification factor f_i is gradually reduced to unity by checking the 'flatness' of the energy histogram; the histogram for all possible E is not less than some value of the average histogram, say, 80%.

We simulate the AF q-state Potts model ($q = 3, 4, 5, 6$) on a simple cubic lattice by using the Wang–Landau algorithm [24]. We impose the periodic boundary conditions and the linear sizes are $L = 8$, 10, 12, 14 and 16. For the modification factor f_i, we start with $f_0 = e^k$ with $k = 1$ or some positive integer, and $f_{i+1} = \sqrt{f_i}$; the final value of $\ln f_i$ is chosen as 10^{-8}, which is the same as [24]. We calculate the density of states $g(E)$, and measure the physical quantities of interest as a function of E. Then, the canonical average of the physical quantity Q at the inverse temperature $\beta = 1/k_{\mathrm{B}}T$ is calculated through the standard relation

$$\langle Q\rangle_\beta = \frac{\int Q(E)g(E)\mathrm{e}^{-\beta E}\,\mathrm{d}E}{\int g(E)\mathrm{e}^{-\beta E}\,\mathrm{d}E}. \tag{9}$$

In the actual calculation, the relative density of states, $g(E_1)/g(E_2)$, is directly obtained. In terms of the entropy (in units of k_{B}), $S(E) = \ln g(E)$, the entropy difference, $S(E_1) - S(E_2)$, is directly measured. Imposing the constraint

$$\sum_E g(E) = q^N \tag{10}$$

we can determine the absolute value of $g(E)$. Here, $N(= L^3)$ is the number of lattice sites, that is the number of Potts spins. For the AF Potts model on a simple cubic lattice, equation (1), the energy E takes a value from zero to $3N$ in units of J. The state with the highest energy $E = 3N$ is nothing but the ferromagnetic ground state, and the degeneracy of the ferromagnetic ground states is q. Therefore, we may check the accuracy of the calculation by confirming $g(3N) = q$.

3. Phase transitions of AF Potts model

First, we study the phase transition of the AF Potts model with $q = 3$, 4, 5 and 6. Let us start with showing the data for $q = 3$ in order to make a comparison with higher-state models, although the phase transition of the three-state Potts model has been studied extensively [6–10]. The temperature dependence of $\langle \boldsymbol{M}^2 \rangle$ for $q = 3$ is shown in figure 1(a). The data for $L = 8$, 10, 12, 14 and 16 are plotted by the dot–dashed, dashed, short-dashed, dotted and solid curves, respectively. The temperature is represented in units of J/k_{B}. All the measurements are made for four independent runs, and the average is taken over four samples. The normalized fourth-order cumulant of the magnetization, the Binder parameter [26]

$$g = \frac{q+1}{2}\left(1 - \frac{q-1}{q+1}\frac{\langle \boldsymbol{M}^4 \rangle}{\langle \boldsymbol{M}^2 \rangle^2}\right) \tag{11}$$

is plotted in figure 1(b). The normalization factors in equation (11) are chosen such that

$$g \to \begin{cases} 1 & \text{for} \quad T = 0 \\ 0 & \text{for} \quad T = \infty \end{cases} \tag{12}$$

by taking account of the $(q-1)$-dimensional vector structure of the order parameter. The definition of equation (11) becomes a usual one for the scalar order parameter ($q = 2$). Since the prefactors of the L dependence in the finite-size scaling equations are cancelled out, one may determine the critical temperature T_{c} from the crossing point of the data of temperature dependence for different sizes as long as the corrections to finite-size scaling are negligible. We also plot the specific heat in figure 1(c). The specific heat peak becomes sharper when the system size is larger. From figures 1(a)–(c), we find a clear phase transition at a finite temperature.

The finite-size scaling plots of the order parameter, and the Binder parameter

$$\langle \boldsymbol{M}^2 \rangle = L^{-2\beta/\nu} f\left((T - T_{\mathrm{c}})L^{1/\nu}\right) \tag{13}$$

$$g = g\left((T - T_{\mathrm{c}})L^{1/\nu}\right) \tag{14}$$

are given in figures 2(a) and (b), respectively. The estimated values for the critical temperature and the critical exponents are $T_{\mathrm{c}} = 1.222(4)$, $1/\nu = 1.52(4)$ and $\beta/\nu = 0.46(5)$. Here, the number in the parentheses denotes the uncertainty in the last digit. The estimated values are consistent with the previous studies [6–9], and the obtained exponents are close to those of the three-dimensional XY model. We have given the estimate using the finite-size scaling analysis to check the consistency of the calculation. Precisely speaking, due to small system sizes, our estimate of T_{c} is a little lower than the accurate estimate [6, 7], which results in a slightly smaller β/ν. To discuss more accurate estimates of T_{c} and the critical exponents, calculations with larger system sizes are preferable.

It is not easy to estimate the specific heat exponent α from the specific heat data using the finite-size scaling analysis if α is negative [6]. We may use the temperature derivative of the specific heat, which is singular at T_{c} even if α is negative. We plot the temperature derivative of the specific heat in figure 3. Since we directly calculate the density of states by using the

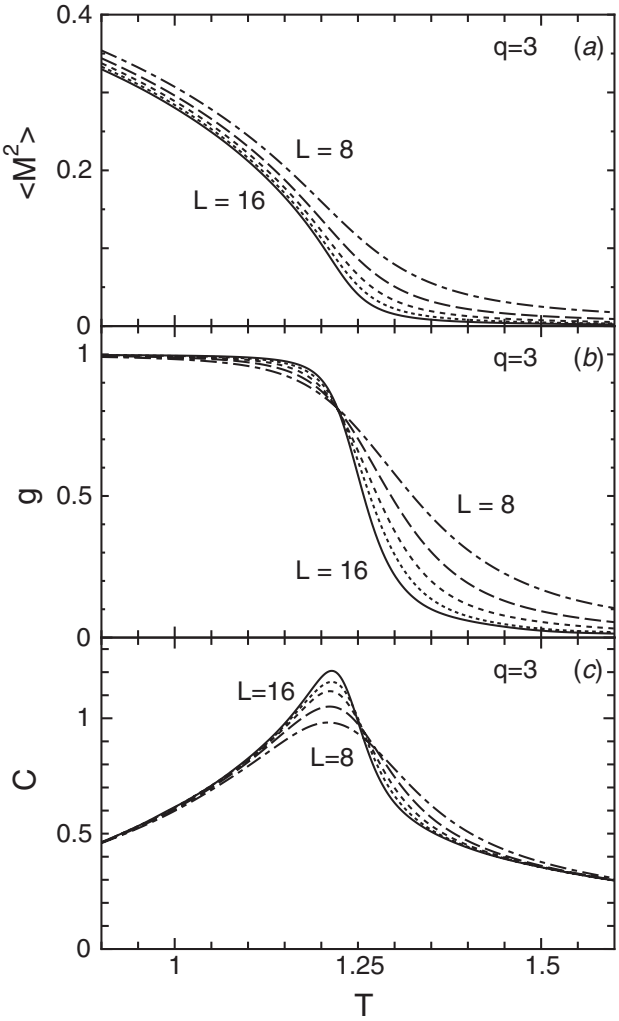

Figure 1. Temperature dependence of the squared order parameter (a), the Binder parameter (b) and the specific heat (c) for the three-dimensional AF three-state Potts model. The linear system sizes are $L = 8$, 10, 12, 14 and 16. The dot–dashed, dashed, short-dashed, dotted and solid curves are used for $L = 8$, 10, 12, 14 and 16, respectively. The temperature is represented in units of J/k_{B}.

Wang–Landau algorithm, it is easy to compute the temperature derivative of the specific heat from the moments of energy. Using the finite-size scaling relation

$$\frac{\mathrm{d}C}{\mathrm{d}T} = L^{(\alpha+1)/\nu} f\left((T - T_{\mathrm{c}})L^{1/\nu}\right) \tag{15}$$

we estimate the exponent α as $-0.04(6)$. Although our estimate has a relatively large error bar due to the small system size, our result suggests that α is negative.

Next we turn to the four-state Potts model. We plot the temperature dependence of the order parameter and the Binder parameter in figures 4(a) and (b), respectively. We also show the specific heat in figure 4(c). We make a comment here on the statistical errors for the estimate of the density of states. They become larger for higher q and larger L. The errors

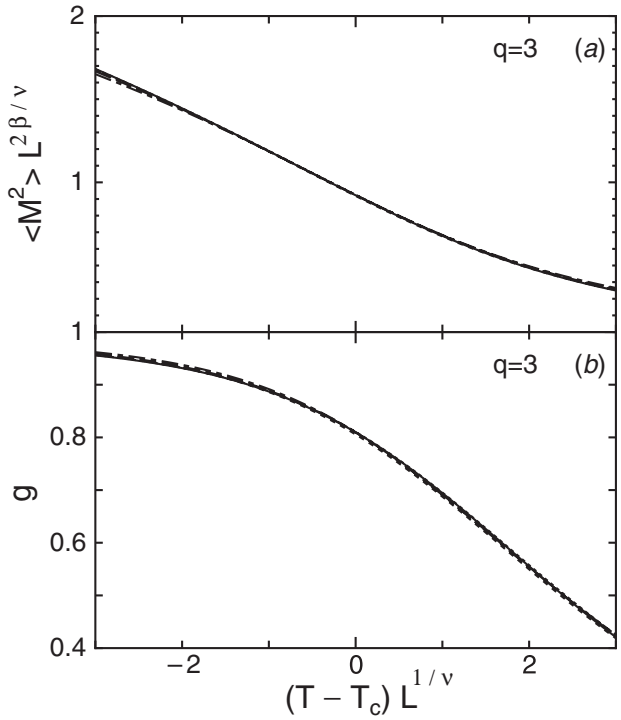

Figure 2. Scaling plots of the order parameter (a) and the Binder parameter (b) for the three-dimensional AF three-state Potts model. The linear system sizes are $L = 8$, 10, 12, 14 and 16. The estimated values for the critical temperature and the critical exponents are $T_c = 1.222$, $1/\nu = 1.52$ and $\beta/\nu = 0.46$.

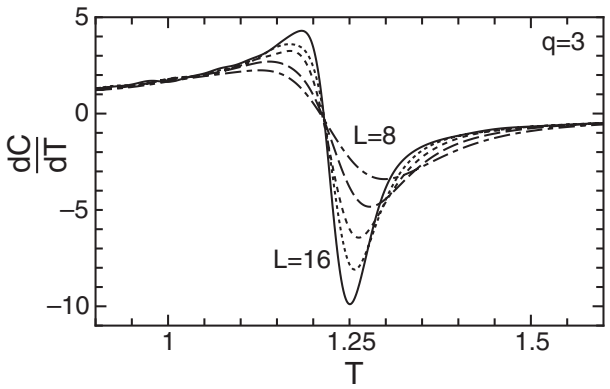

Figure 3. Temperature derivative of the specific heat for the three-dimensional AF three-state Potts model. The linear system sizes are $L = 8$, 10, 12, 14 and 16.

for the specific heat curve for larger L are larger than the thickness of the curve in figure 4(c). From figure 4 we find that there exits a clear finite-temperature phase transition. The finite-size scaling plots of the order parameter and the Binder parameter are given in figures 5(a) and (b), respectively; we estimate T_c, $1/\nu$ and β/ν as 0.669(4), 1.41(4) and 0.44(6). These are

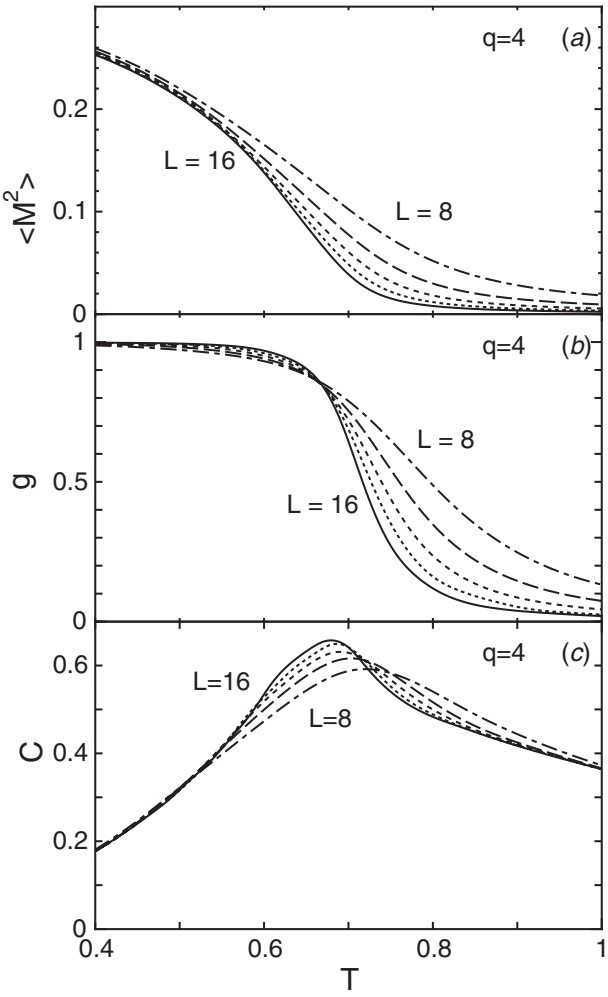

Figure 4. Temperature dependence of the squared order parameter (a), the Binder parameter (b) and the specific heat (c) for the three-dimensional AF four-state Potts model. The linear system sizes are $L = 8$, 10, 12, 14 and 16. The temperature is represented in units of J/k_{B}.

compatible with the previous study [12], and the obtained exponents are close to those of the three-dimensional Heisenberg model. Precisely, our estimate of T_{c} is a little lower than the accurate estimate [12]; the situation is the same as the case of $q = 3$.

The order parameter, the Binder parameter and the specific heat for the five-state Potts model are given in figures 6(a)–(c), respectively. There is no anomaly in the specific heat. There is no crossing in the Binder parameter at finite temperatures. The critical temperature is down to zero. However, the value of the Binder parameter at $T = 0$ is finite, and it may become constant for large enough L; it is not clear whether $T = 0$ is critical or not. To determine this point, more elaborate studies with larger sizes are necessary.

We show the order parameter, the Binder parameter and the specific heat for the six-state Potts model in figures 7(a)–(c), respectively. In this case, the maximum linear size is $L = 14$. There is no anomaly in the specific heat. The value of the Binder parameter at $T = 0$ is very

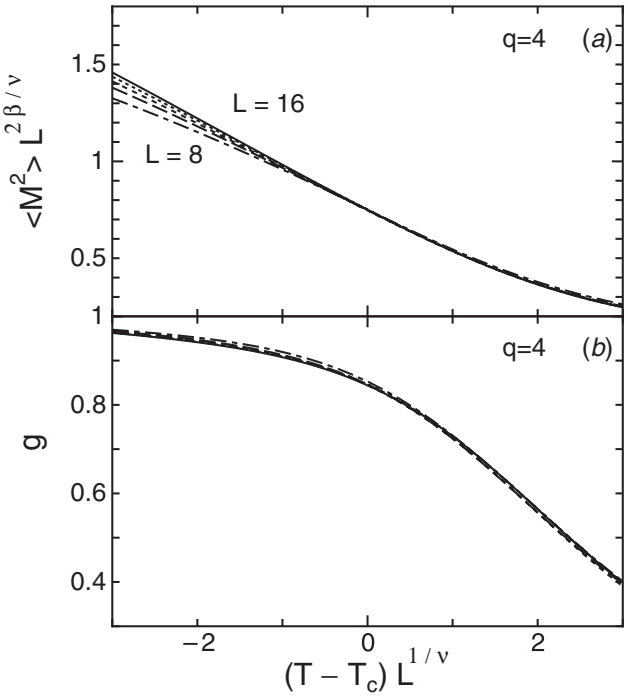

Figure 5. Scaling plots of the order parameter (*a*) and the Binder parameter (*b*) for the three-dimensional AF four-state Potts model. The linear system sizes are $L = 8$, 10, 12, 14 and 16. The estimated values for the critical temperature and the critical exponents are $T_c = 0.669$, $1/\nu = 1.41$ and $\beta/\nu = 0.44$.

small. This means that the distribution of the order parameter is Gaussian; in other words, the system is disordered. We may conclude that there is no order even at $T = 0$.

4. Ground-state properties

In this section, we focus on the ground-state properties of the AF Potts models. First, we consider the ground-state entropy per spin, S_0/N; the entropy (in units of k_B) is calculated through $S_0 = \ln g(0)$.

In figure 8, we show the size dependence of the ground-state entropy per spin for the q-state AF Potts model on a simple cubic lattice. We plot S_0/N as a function of $1/N$, and find a linear $1/N$ dependence. Using the least-squares method, for $q = 3$ we have

$$S_0/N = 0.3670(1) + 1.97(4) \times (1/N) \qquad q = 3 \tag{16}$$

where the number in the parentheses denotes the uncertainty in the last digit. Wang *et al* [6] estimated the ground-state entropy per spin ($N \to \infty$) as 0.3673 from the data of $L = 4$ and 8. Our estimate, 0.3670, is a little smaller than their estimate. The low-temperature phase of the AF three-state Potts model is the BSS state. The typical configuration of the BSS state is that all the spins on the sublattice A take one of the three states, and the spins on sublattice B take one of the other two states randomly. Then, the lower bound for the ground-state entropy becomes $S_0/N \geqslant (\ln 2)/2 + \ln 6 \times (1/N) = 0.3466 + 1.79 \times (1/N)$. Our estimate, equation (16), is, of course, larger than the lower bound. That is, there are many configurations other than the typical configurations of the BSS state.

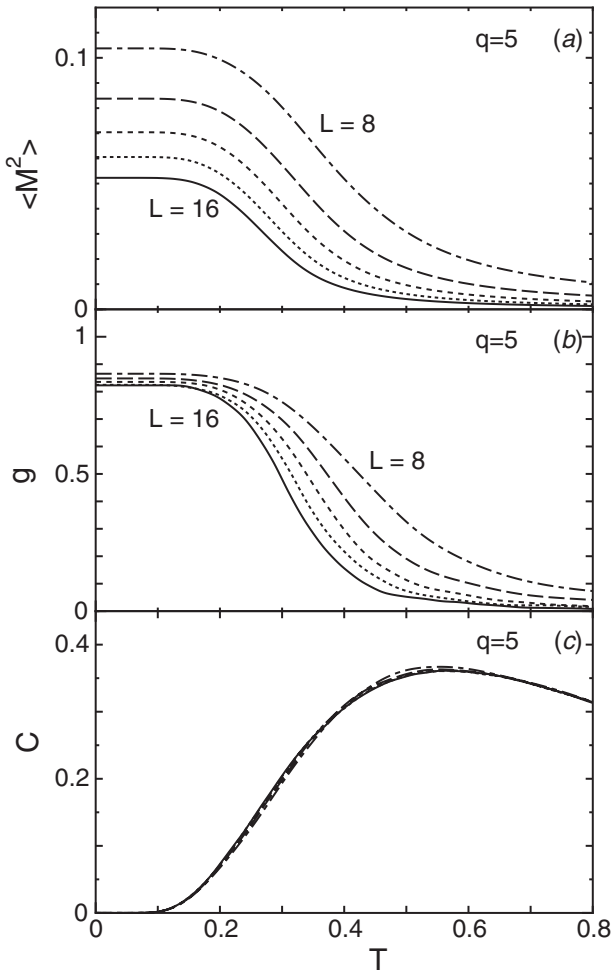

Figure 6. Temperature dependence of the squared order parameter (*a*), the Binder parameter (*b*) and the specific heat (*c*) for the three-dimensional AF five-state Potts model. The linear system sizes are $L = 8$, 10, 12, 14 and 16. The temperature is represented in units of J/k_B.

From the linear $1/N$ dependence for the AF four-state Potts model, we have

$$S_0/N = 0.7148(1) + 1.92(6) \times (1/N) \qquad q = 4. \tag{17}$$

As far as we know, there has been no study on the estimate of the ground-state entropy for $q = 4$ and higher q. For the low-temperature phase of the four-state Potts model, the typical spin configuration is as follows: the spins on sublattice A take two of four states randomly, whereas those on sublattice B take the other two states. Then, the lower bound for the ground-state entropy becomes $S_0/N \geqslant \ln 2 + \ln 6 \times (1/N) = 0.6931 + 1.79 \times (1/N)$. Our estimate, equation (17), is again larger than the lower bound.

From the size dependence of the ground-state entropy for the AF five-state Potts model, which is also shown in figure 8, we have

$$S_0/N = 0.9997(1) + 2.03(6) \times (1/N) \qquad q = 5. \tag{18}$$

The main contribution to the low-temperature phase of the five-state Potts model is as follows: the spins on sublattice A take two of five states randomly, whereas those on sublattice B

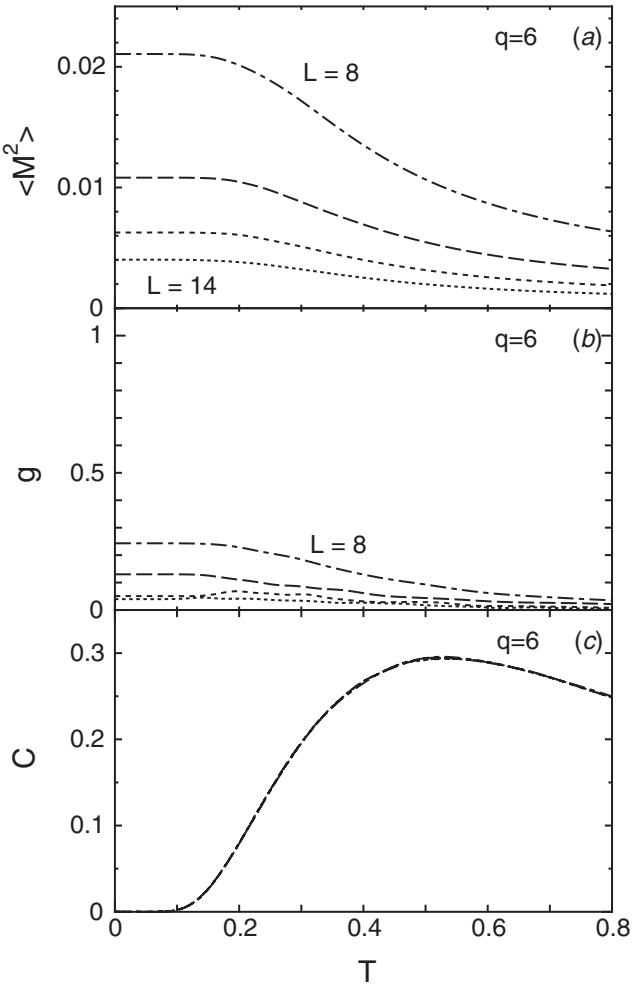

Figure 7. Temperature dependence of the squared order parameter (*a*), the Binder parameter (*b*) and the specific heat (*c*) for the three-dimensional AF six-state Potts model. The linear system sizes are $L = 8$, 10, 12 and 14. The temperature is represented in units of J/k_B.

take the other three states. Then, the lower bound for the ground-state entropy becomes $S_0/N \geqslant (\ln 6)/2 + 2\ln 5 \times (1/N) = 0.8959 + 3.00 \times (1/N)$. Our estimate, equation (18), is again larger than the lower bound.

Finally, for $q = 6$ we have

$$S_0/N = 1.2717(1) + 0.17(4) \times (1/N) \qquad q = 6 \tag{19}$$

by using the least-squares method. The main contribution of the six-state Potts model is as follows: the spins on sublattice A take three of six states randomly, whereas those on sublattice B take the other three states. Our estimate, equation (19), is again larger than the lower bound for the ground-state entropy; $S_0/N \geqslant \ln 3 + 2\ln 5 \times (1/N) = 1.0986 + 3.00 \times (1/N)$.

It is interesting to note that the ground-state entropy has a similar $1/N$ dependence for all $q = 3$, 4 and 5, although there occurs a finite-temperature phase transition for $q = 3$ and 4

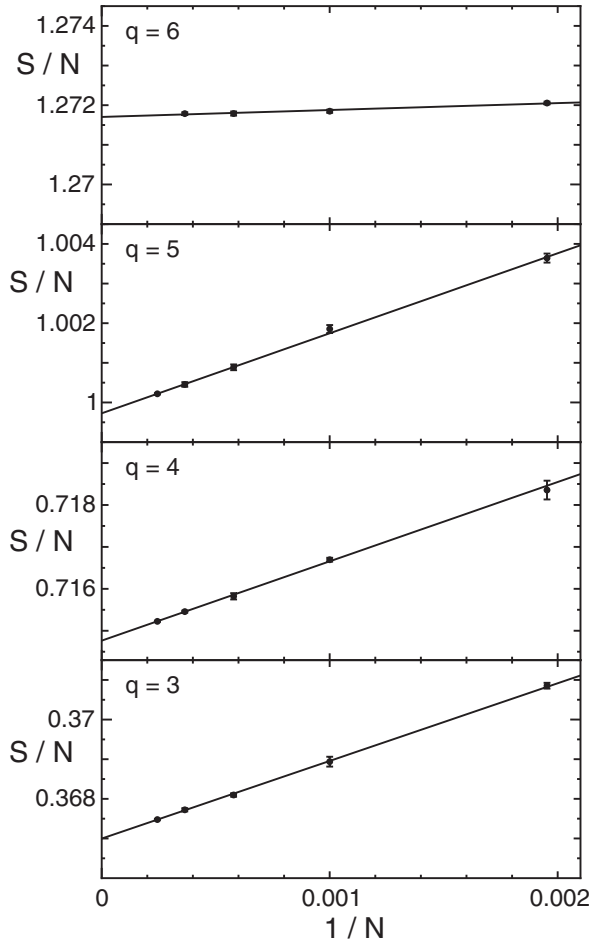

Figure 8. Size dependence of the ground-state entropy per spin for the three-dimensional AF q-state Potts models; $q = 3$, 4, 5 and 6. The linear system sizes are $L = 8$, 10, 12, 14 and 16 for $q = 3$–5 and $L = 8$, 10, 12 and 14 for $q = 6$; $N = L^3$.

and a zero-temperature phase transition for $q = 5$. The size dependence of $q = 6$ is similar to that for $q = 3$, 4 and 5, but the slope of the $1/N$ dependence for $q = 6$ is smaller than that of others. It is not clear whether this small difference is related to the existence of the AF order.

We find that the ground-state entropy is larger than the contribution from the typical configurations of the BSS state. In order to look into the ground-state properties more carefully, let us consider the proportion of visiting the typical BSS ground states among all the ground states. As an example, we treat the case of $q = 3$. Since this proportion becomes very small for larger sizes, we have checked it for a smaller system, that is, $L = 6$. The estimate of the ground-state entropy per spin S_0/N for $L = 6$ is 0.376. Thus, the expected value for the proportion of the typical BSS ground states among all the ground states is $6 \cdot 2^{(N/2)}/\mathrm{e}^{0.376N} = 0.010$ ($N = 216$). Actually, the typical BSS ground states were visited 0.010 times as frequently as all the ground states, which is consistent with the theoretical expectation. In other words, we sample ground states uniformly.

Next we study the distribution of the ground states. As an example, we again deal with the

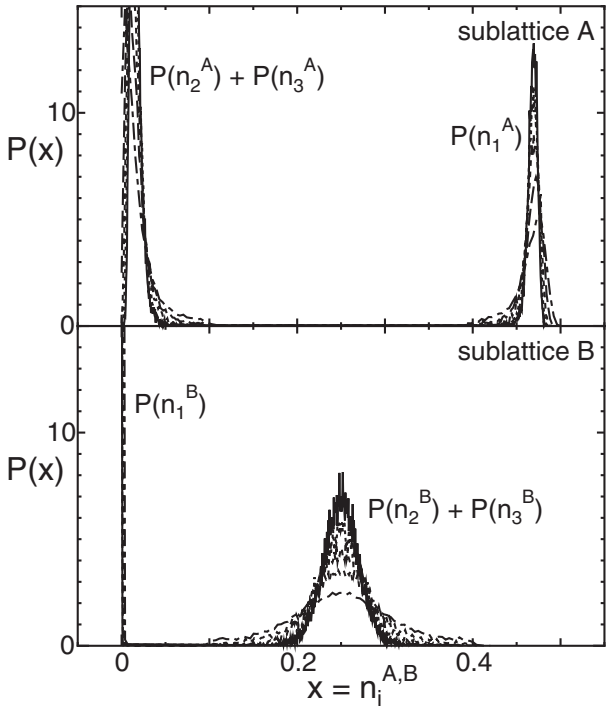

Figure 9. Distribution function $P(x)$ for the ground states of the three-dimensional AF 3-state Potts models. Here x stands for $n_i^{\mathrm{A,B}}$ $(i = 1, 2, 3)$, the number of each component per spin on sublattice A or B. The linear system sizes are $L = 8$, 10, 12, 14 and 16. The same types of curve for different sizes are used as in figure 1.

case of $q = 3$. Let us denote the number of each component per spin as $n_i^{\mathrm{A,B}}$ $(i = 1, 2, 3)$; then

$$0 \leqslant n_i \leqslant 1/2 \qquad \text{and} \qquad m_i = n_i^{\mathrm{A}} - n_i^{\mathrm{B}} \tag{20}$$

where the staggered magnetization m_i is given in equation (2). We show the distribution function of $n_i^{\mathrm{A,B}}$ for $L = 8$, 10, 12, 14 and 16 in figure 9. The same types of curve for different sizes are used as in figure 1. The distribution is sharper for larger sizes. In plotting the data in figure 9, we have chosen component 1 and sublattice A such that n_1^{A} is the largest. The distribution function $P(n_i^{\mathrm{A,B}})$ is normalized such that

$$\int P(n_i^{\mathrm{A,B}})\,\mathrm{d}n_i^{\mathrm{A,B}}$$

is independent of the size. For the typical BSS states, we expect the δ-function distribution for sublattice A, $P(n_1^{\mathrm{A}}) = \delta(n_1^{\mathrm{A}} - 1/2)$, $P(n_{2,3}^{\mathrm{A}}) = \delta(n_{2,3}^{\mathrm{A}})$; $P(n_2^{\mathrm{B}}) + P(n_3^{\mathrm{B}})$ becomes the Gaussian distribution around $1/4$ and $P(n_1^{\mathrm{B}}) = \delta(n_1^{\mathrm{B}})$ for sublattice B. Our results shown in figure 9 are close to those of the typical BSS states, but we can see a clear deviation from the typical BSS states and the size dependence. In other words, there are many configurations other than the typical configurations of the BSS state. Similar behaviour is also obtained for the ground states of higher-state Potts models. The deviation from the typical BSS states becomes larger for higher q.

5. Summary and discussions

To summarize, we have applied a newly proposed Monte Carlo algorithm, the Wang–Landau algorithm [24], to the study of the three-dimensional AF q-state Potts models. We obtain the finite-temperature phase transition for $q = 3$ and 4, whereas the transition temperature is down to zero for $q = 5$. For $q = 6$ there exists no order for any temperature. We also study the ground-state properties. From the analysis of the size dependence of the ground-state entropy, we find that the ground-state entropy is larger than the contribution from the typical configurations of the BSS state for $q = 3$. The same situations are found for $q = 4$, 5 and 6.

We have confirmed again the efficiency of the Wang–Landau algorithm. For the study of only the critical phenomena near the critical point, other methods may have advantages. However, in order to make a systematic study for the whole energy space, we can treat larger systems by using the Wang–Landau algorithm, especially for higher-q-state Potts models.

In the present paper we have studied the ground-state entropy for the three-dimensional AF Potts models. We had better mention that the accurate estimate of the nonzero ground-state entropy is easily obtained for the two-dimensional AF Potts models, of course; the obtained data are consistent with the previous studies [13]. It is also interesting to apply the Wang–Landau algorithm to the systematic study of both the ground-state properties and the phase transitions for more complicated systems, such as spin glass problems.

Acknowledgments

We thank N Kawashima, H Otsuka, M Kikuchi and F Wang for valuable discussions. The computation in this work has been performed using the facilities of the Supercomputer Center, Institute for Solid State Physics, University of Tokyo. This work was supported by a Grant-in-Aid for Scientific Research from the Ministry of Education, Science, Sports and Culture, Japan.

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