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Critical behaviour of the ferromagnetic Ising model on a triangular lattice*

Luo Zhi-Huan(罗志环)[a)b)], Loan Mushtaq[c)],
Liu Yan(刘 岩)[a)†], and Lin Jian-Rong(林健荣)[d)]

[a)] *Department of Applied Physics, South China Agricultural University, Guangzhou* 510642, *China*
[b)] *Department of Physics, Sun Yet-Sen University, Guangzhou* 510275, *China*
[c)] *International School, Jinan University, Guangzhou* 510632, *China*
[d)] *Engineering College, South China Agricultural University, Guangzhou* 510642, *China*

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We use a new updated algorithm scheme to investigate the critical behaviour of the two-dimensional ferromagnetic Ising model on a triangular lattice with the nearest neighbour interactions. The transition is examined by generating accurate data for lattices with $L = 8$, 10, 12, 15, 20, 25, 30, 40 and 50. The updated spin algorithm we employ has the advantages of both a Metropolis algorithm and a single-update method. Our study indicates that the transition is continuous at $T_c = 3.6403(2)$. A convincing finite-size scaling analysis of the model yields $\nu = 0.9995(21)$, $\beta/\nu = 0.12400(17)$, $\gamma/\nu = 1.75223(22)$, $\gamma'/\nu = 1.7555(22)$, $\alpha/\nu = 0.00077(420)$ (scaling) and $\alpha/\nu = 0.0010(42)$ (hyperscaling). The present scheme yields more accurate estimates for all the critical exponents than the Monte Carlo method, and our estimates are shown to be in excellent agreement with their predicted values.

Keywords: Ising model, triangular lattice, Monte Carlo method
PACC: 0550, 0570

1. Introduction

The Ising model on a triangular lattice, as an archetypical example of a frustrated system, was initially studied by Wannier[1] and Newell.[2] The triangular Ising model has attracted much attention because of its remarkable properties, and it has a long history of investigation. No exact solution is available in two dimensions in an arbitrary magnetic field. Hence, the simulation of the Ising model is essential. Monte Carlo simulation methods have been widely used as a technique to update the spins of the system and to study the Ising model on a triangular lattice to obtain numerical solutions.

A number of Monte Carlo methods based on Metropolis algorithms[3] have been applied to the model in the past and yielded somewhat mixed results. A classical Monte Carlo using the Metropolis algorithm runs into difficulties on large lattice sizes due to critical slowing down and rapid increase in the correlation time. Because of these reasons it is difficult to obtain meaningful results on larger lattice sizes. A cluster technique, in which a multi-cluster algorithm is used, was pioneered by Swendsen and Wang.[4] Their method successfully demonstrated its validity and efficiency for the Potts model. Similar ideas have been pursued by Wolf[5] who proposed a single-cluster algorithm, the algorithm that is a nonlocal updating technique based on a multiple-cluster algorithm but more efficient and easier to achieve the meaningful results. Both of these cluster algorithms are very effective in reducing critical slowing down. But for the same system, one sweep of a single-cluster or multiple-clusters takes much more time than that taken by the Metropolis algorithm, hence these methods are less effective for large lattice sizes. Very little work has been done since then on using these approaches to this model. Because large systems have the advantage of reducing finite-size effects, we have to look yet again for an alternative approach.

In the present study, we attempt to use a mixture of a single-cluster (multiple-cluster) algorithm and a Metropolis algorithm, which are both extended to the Ising model in two dimensions on a triangular lattice. Applications of the combined algorithm tech-

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†Corresponding author. E-mail: lycalm@scau.edu.cn

nique have been extremely successful in lattice quantum chromodynamics (QCD)[6−12] and have given rise to great optimism about the possibility of obtaining results relevant to continuum physics from Monte Carlo simulations of the lattice version of the corresponding theory. As mentioned above, our aim is to use standard Monte Carlo techniques based on the combined function of a single-cluster (multiple-cluster) and a Metropolis algorithm to update the spins of the system and see whether useful results can be obtained. The values of the critical exponents are well established for this model in two dimensions, and in order to prove that our method is successful, these well-established values must be reproduced. For this purpose, the critical exponents are computed by using the combined algorithm.

The rest of the present paper is organised as follows. In Section 2 we discuss the Ising model in two dimensions in its lattice formulation. Here we describe the details of the simulations and the methods used to extract the observables. We present and discuss our results in Section 3. Our conclusions are finally given in Section 4.

2. Model and simulation details

The Hamiltonian of the model is given by

$$H = -J \sum_{<i,j>} S_i S_j, \tag{1}$$

where J is positive and denotes the strength of ferromagnetic interaction, $S_i = \pm 1$ are the Ising spin variables, and $< i, j >$ restricts the summation to distinct pairs of the nearest neighbours. The geometrical structure of the model is shown in Fig.1. Periodic boundary conditions are employed in simulation to reduce the finite-size effects.

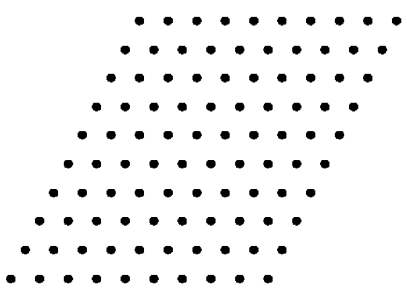


Fig.1. Triangular Ising net.

Configuration ensembles are generated by using the mixed algorithm of the Metropolis and single-cluster (multiple-cluster) methods on a two-dimensional triangular lattice of size $L = 8 - 50$. We outline the procedure of the single-cluster updating algorithm used to study the Ising model on a triangular lattice below.

(a) Choose a random lattice site x as the first point of cluster c to be built.

(b) Visit all sites directly connecting to x, and add them to the cluster c with probability $P(S_x, S_y) = 1-\exp\{\min[0, 2KS_xS_y]\}$, where y is the nearest neighbour of site x and K is the reciprocal of temperature.

(c) Continue iteratively in the same way for the newly adjoined sites until the process stops.

(d) Flip the all sites of the cluster c.

(e) Repeat steps (a), (b), (c) and (d) sufficiently.

We define a compound sweep as one single-cluster updating sweep followed by five Metropolis updating sweeps. In our simulations, five compound sweeps are performed between measurements. We can find that the Metropolis-single-cluster (multiple-cluster) and compound sweep updating techniques are equally good for large ensembles. However, in the case of the compound sweep technique the computational cost turns out to be far less. For this reason we adopt this technique in our simulations.

We generate 1×10^7 ensembles at a transition point for each lattice size to perform the finite-size analysis. High statistics can help obtain a more accurate result. Since the ensembles are generated by using the Monte Carlo method, they are not completely uncorrelated with each other. The Jackknife procedure is employed because it takes the autocorrelation between the ensembles into account and improves estimates of mean values and errors.

3. Results and discussion

From the fluctuation dissipation theorem, the heat capacity (C) is the derivative of the energy with respect to temperature and has the form

$$C = \frac{\langle E^2 \rangle - \langle E \rangle^2}{L^2 T^2}. \tag{2}$$

For improving the comparability among different system sizes, it is better to compute the heat capacity per spin which is displayed in Fig.2. Theoretical derivations suggest that the heat capacity should behave like $\log |T - T_c|$ near the critical temperature. We notice a progressive steepening of the peak as the lattice size increases, which illustrates a more apparent phase

transition. Note that due to finite size effects, the peak is flattened and moved to the right. Our interest is to look for such a transition point and investigate the critical phenomena associated with the transition by using the finite-size scaling method.[13−15]

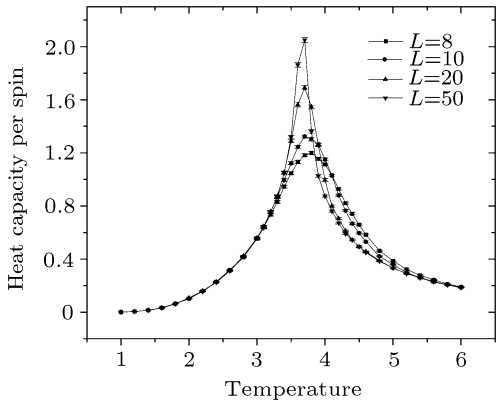


Fig.2. Curves for heat capacity with respect to temperature for four different lattice sizes, $L \times L$.

3.1. Estimation of transition temperature

The fourth-order magnetic cumulant, which is used to estimate the transition temperature, is defined by the following expression:[15]

$$U(T,L) = 1 - \frac{\langle m^4(T,L)\rangle}{3\langle m^2(T,L)\rangle^2}, \tag{3}$$

where $\langle m^k(T,L)\rangle$ is the thermodynamic average value of the kth power of the magnetic order parameter per spin for the lattice of size L at temperature T. The variation of $U(T;L)$, for a given size L, with temperature is illustrated in Fig.3. To determine the temperature $T_c(L,L')$, we make use of the condition[15,16]

$$\left.\frac{U(T,L')}{U(T,L)}\right|_{T=T_c(L,L')} = 1, \tag{4}$$

where L' and L are two different lattice sizes. Thus we can determine $T_c(L,L')$ by locating the interaction of these curves - the so-called 'cumulant crossing'.

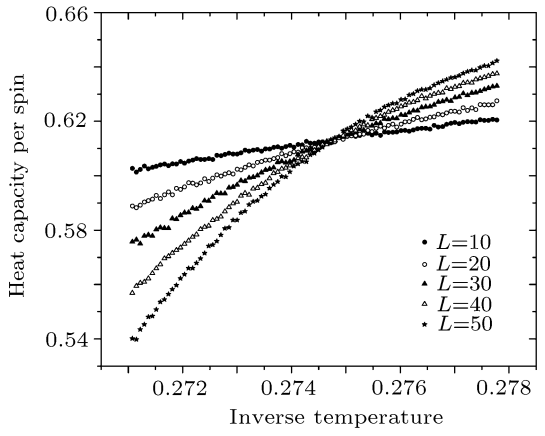


Fig.3. Curves for fourth-order magnetic parameter cumulant versus the reciprocal of temperature for five different lattice sizes.

Figure 4 shows the results for $T_c(L,L')$ plotted as a function of the ratio $\ln^{-1}(L'/L)$. Keeping L fixed, linear extrapolation is performed to obtain $T_c(L,\infty)$ which corresponds to the critical temperature of lattice size L. Results of the extrapolations for $8 \le L \le 15$ accord quite well within the errors. The transition temperature for the infinite lattice, T_c, is thus estimated as 3.6403(2), i.e. $T_c = 3.6403(2)$, which is much closer to the exact value $4/\ln 3$.

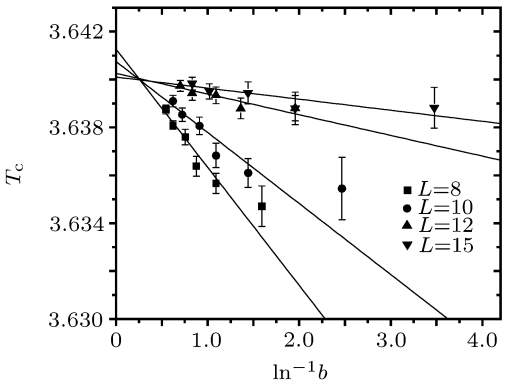


Fig.4. Estimates for T_c versus the reciprocal of logarithm of scale factor $b = L'/L$ for four different lattice sizes.

3.2. Order of transition

A better way to identify the order of transition is the internal-energy cumulant[17−22] defined as

$$V(T,L) = 1 - \frac{\langle E^4(T,L)\rangle}{3\langle E^2(T,L)\rangle^2}, \tag{5}$$

where $\langle E^k(T,L)\rangle$ is the thermodynamic average value of kth power of internal energy for the lattice of size L at temperature T. $V(T,L)$ is a useful quantity since its behaviour at a continue phase transition is quite different from that at a first order transition. This variable has a minimum (near the critical point) and in the limit $L \to \infty$ achieves the value $V^* = \frac{2}{3}$ for a continuous transition, whereas $V^* < \frac{2}{3}$ is expected in the case of a first-order transition. Plots of $V(T,L)$

versus temperature for several lattice sizes are shown in Fig.5, indicating that the transition is not of the first-order since the energy culumant $V(T, L)$ does not peak near the critical temperature. This has also been observed in other studies.[19,21,22]

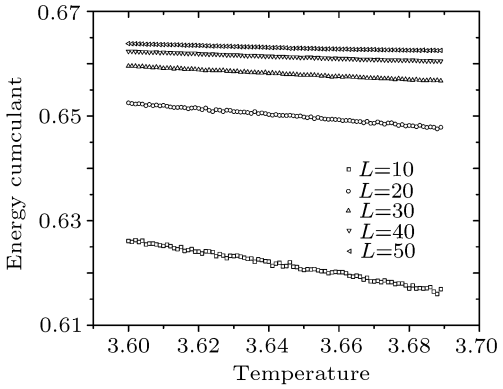


Fig.5. Curves for energy cumulant with respect to temperature for five different lattice sizes.

Figure 6 shows the order parameter cumulant $U(T, L)$ as a function of temperature for several lattice sizes. In contrast with obtaining a negative minimum value in first order transition, $U(T, L)$ drops from 2/3 for $T < T_c$ to 0 for $T > T_c$. This is consistent with the continuous transition.[17]

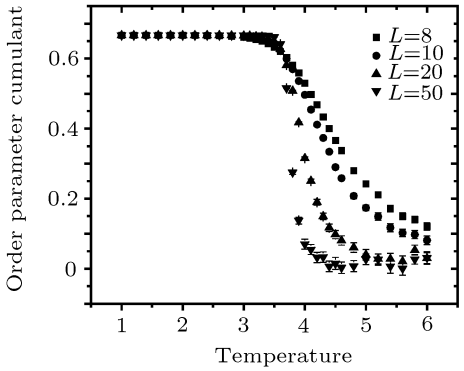


Fig.6. Curves for order parameter cumulant with respect to temperature for four different lattice sizes.

Since the magnetic susceptibility χ scales as L^d for a discontinuous transition and as $L^{\gamma/\nu}$ for a continuous one,[23] we can also determine the transition order from χ scaling behaviours. As discussed below, we find that χ scales as $L^{1.75223}$ for $T < T_c$ and as $L^{1.7555}$ for $T > T_c$, but not as L^2. Thus we can conclude that the transition is continuous.

3.3. Estimation of critical exponents

To estimate critical exponents, finite-size scaling relations at the critical point are used. For this purpose, we extract the critical exponents, which are related to specific heat, the order parameter, and the susceptibility, from our simulation data at $T_c(\infty)$ by using finite-size analysis.[13–15]

First we extract ν from $\mathrm{d}U/\mathrm{d}K$ which obeys the following relation:

$$\frac{\mathrm{d}U}{\mathrm{d}K} \sim L^{1/\nu}. \tag{6}$$

The finite-difference derivative method can be used to determinate $\mathrm{d}U/\mathrm{d}K$, but it is rather a poor choice since the results are highly sensitive to the interval of the linear approximation. To obtain an accurate result of the critical exponent ν, one can write the derivative of U with respect to K as

$$\begin{aligned}\frac{\mathrm{d}U}{\mathrm{d}K} &= \frac{1}{3\langle m^2\rangle^2}\left[\langle m^4\rangle\langle E\rangle - 2\frac{\langle m^4\rangle\langle m^2E\rangle}{\langle m^2\rangle} + \langle m^4E\rangle\right] \\ &= \left\langle \frac{m^4(\langle E\rangle - E)}{3\langle m^2\rangle^2}\right\rangle - \left\langle \frac{2m^2E\langle m^4\rangle}{3\langle m^2\rangle^3}\right\rangle. \end{aligned} \tag{7}$$

The plot of $\ln(\mathrm{d}U/\mathrm{d}K)$ versus $\ln L$ is shown in Fig.7. The slope of the straight line obtained from the log–log plot of the scaling relation corresponding to this quantity gives the correlation length exponent $\nu = 0.9995(21)$, which is slightly different from the exact value. Since the critical properties of $\ln(\mathrm{d}U/\mathrm{d}K)$ have a large lattice size dependence,[24] we can also extract the value of ν from other observables, which are defined as follows:[23–25]

$$\begin{aligned} V_1 &= \ln\left[\frac{\mathrm{d}\ln\langle m\rangle}{\mathrm{d}K}\right] = \ln\left[\langle E\rangle - \frac{\langle mE\rangle}{\langle m\rangle}\right] \\ &= \ln\left\langle \frac{E(\langle m\rangle - m)}{\langle m\rangle}\right\rangle, \end{aligned} \tag{8}$$

$$V_2 = \ln\left[\frac{\mathrm{d}\ln\langle m^2\rangle}{\mathrm{d}K}\right] = \ln\left\langle \frac{E(\langle m^2\rangle - m^2)}{\langle m^2\rangle}\right\rangle, \tag{9}$$

$$V_3 = 2[m] - [m^2], \tag{10}$$

and

$$V_4 = 3[m^2] - 2[m^3], \tag{11}$$

where

$$\begin{aligned}[m^n] &= \ln\frac{\partial\langle m^n\rangle}{\partial K} \\ &= \ln(\langle E\rangle\langle m^n\rangle - \langle m^nE\rangle) \\ &= \ln\langle E(\langle m^n\rangle - m^n)\rangle. \end{aligned} \tag{12}$$

The curves show a smooth behaviour, and a linear fitting of the data is adopted. We have found that the

slopes of the straight lines of V_i, with $i = 1, 2, 3, 4$, are very close to that of $\ln(\mathrm{d}U/\mathrm{d}K)$ as illustrated in Fig.7.

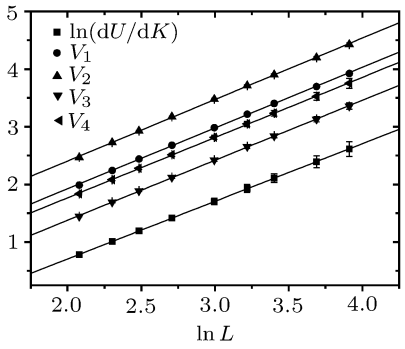


Fig.7. Values of critical exponent ν, determined from the slope of $\ln(\mathrm{d}U_L/\mathrm{d}K)$ and V_i, versus $\ln L$ at $T = 3.6403$, where linear fittings lead to $\nu = 0.9995(21)$.

Figure 8 displays the double-logarithmic plot of the magnetization at the transition point as a function of L. According to the standard theory of finite-size scaling, at T_c the magnetization per spin should obey the relation

$$m \sim L^{-\beta/\nu} \tag{13}$$

for sufficiently large lattice size. The data falls nicely on a linear curve and the slope of the curve gives an estimate for the ratio of critical exponents $\beta/\nu = 0.12400(17)$. Using our estimate of $\nu = 0.9995(21)$, we obtain the critical exponent of magnetization $\beta = 0.12394(32)$.

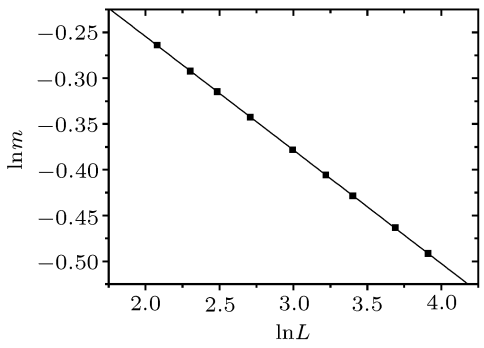


Fig.8. $\ln m$ as a function of $\ln L$ at $T = 3.6403$

On finite lattices, the magnetic susceptibility per spin is given by[16,26]

$$\chi = (L^2/T)\langle m^2 \rangle \tag{14}$$

for $T > T_\mathrm{c}$ and

$$\chi' = (L^2/T)(\langle m^2 \rangle - \langle m \rangle^2) \tag{15}$$

for $T < T_\mathrm{c}$, which satisfy

$$\chi \sim L^{\gamma/\nu} \quad \text{and} \quad \chi' \sim L^{\gamma'/\nu}. \tag{16}$$

As another estimation, we compute the magnetic susceptibility per spin by separately examining the plots of $\ln\chi - \ln L$ and $\ln\chi' - \ln L$ at the transition point as shown in Fig.9. The data display a smooth scaling behaviour. The slope of the linear fitting to the data gives estimates of $\gamma/\nu = 1.75223(22)$ and $\gamma'/\nu = 1.7555(22)$, respectively. With our estimated values $\nu = 0.9995(21)$, we obtain $\gamma = 1.7514(37)$ and $\gamma' = 1.7546(43)$ respectively. These results accord very well with the theoretical predictions.

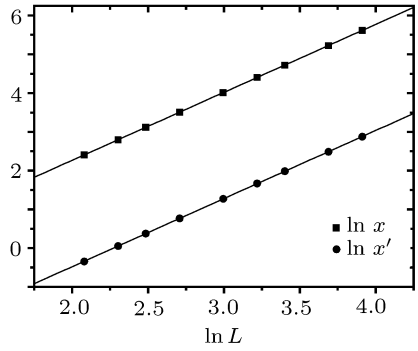


Fig.9. $\ln\chi$ and $\ln\chi'$ versus $\ln L$ at $T = 3.6403$.

With three critical exponents ν, γ and β determined, the fourth exponent α may be estimated by using the following scaling law:

$$2\beta + \alpha + \gamma = 2, \tag{17}$$

thereby yielding $\alpha/\nu = 0.00077(420)$ and $\alpha = 0.00077(420)$ for $\gamma/\nu = 1.75223(22)$, $\alpha/\nu = -0.0025(47)$ and $\alpha = -0.0025(47)$ for $\gamma'/\nu = 1.7555(22)$. We can also estimate α from hyperscaling relation

$$d\nu + \alpha = 2, \tag{18}$$

where $d = 2$ is the dimension of the system. It gives $\alpha = 0.0010(42)$ and $\alpha/\nu = 0.0010(42)$, which are consistent with those given by scaling law.

Estimates of critical exponents from finite-size scaling at critical temperature T_c are summarized in Table 1.

Table 1. Estimates of critical exponents.

exponent	value	exact value[27,28]
ν	0.9995(21)	1
β/ν	0.12400(17)	1/8
γ/ν	1.75223(22)($T > T_c$)	7/4
γ'/ν	1.7555(22)($T < T_c$)	7/4
α/ν	0.00077(420)(by scaling)	0
α/ν	0.0010(42)(by hyperscaling)	0

To ensure the validity of our estimate of α we compare it with those obtained by using the specific heat per spin from the fluctuations of the total energy. For a continuous transition it behaves as

$$C = a + bL^{\alpha/\nu}. \tag{19}$$

Using $\alpha/\nu = 0.00077(420)$ calculated above, the heat capacity at critical temperature is plotted as a function of $L^{0.00077}$ in Fig.10. It is found that the evaluations of expressions (16) and (18) yield very consistent results within statistical errors. We find that the values are in good agreement with the theoretical ones. An overall error of about 0.1%–0.8% is estimated for the values of the critical exponents.

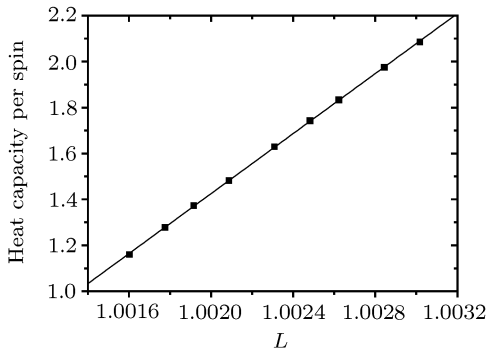


Fig.10. Heat capacity C with respect to $L^{\alpha/\nu}$, where $\alpha/\nu = 0.00077$ and C is evaluated at $T = 3.6403$.

4. Conclusions

We have obtained critical exponents for the Ising model with nearest-neighbour interactions on a triangular lattice by using a mixture of single-cluster and Metropolis algorithms in our simulations. The data are analysed according to finite-size scaling theory. The idea of using extensions of mixed algorithm to estimate the critical exponents seems to supply quite an accurate route to their estimation. In conclusion, it can be stated that the compound update algorithm method with periodic boundary conditions reproduces at a high accuracy the critical properties of the model and confirms the prediction that the first order transition is not supported by the finite size behaviour of the system. Our results show that the estimations of the critical exponents are in good agreement with their theoretical values. We stress that the present result for the exponent is better than the previous estimates obtained by finite size scaling and the Monte Carlo approach.

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References

[1] Wannier G H 1950 *Phys. Rev.* **79** 357

[2] Newell G F 1950 *Phys. Rev.* **79** 876

[3] Metropolis N, Rosenbluth A W, Rosenbluth M N, Teller A H and Teller E 1953 *J. Chem. Phys.* **21** 1087

[4] Swendsen R H and Wang J S 1987 *Phys. Rev. Lett.* **58** 86

[5] Wolf U 1989 *Phys. Rev. Lett.* **62** 361

[6] Morningstar C J and Peardon M 1997 *Phys. Rev.* D **56** 4043

[7] Morningstar C J and Peardon M 1999 *Phys. Rev.* D **60** 034509

[8] Loan M, Luo X Q and Luo Z H 2006 *Int. J. Mod. Phys.* A **21** 2905

[9] Luo Z H, Loan M and Luo X Q 2007 *Mod. Phys. Lett.* A **22** 591

[10] Loan M, Luo Z H and Lam Y Y 2008 *Eur. Phys. J.* C **57** 579

[11] Loan M 2008 *Eur. Phys. J.* C **54** 475

[12] Loan M and Ying Y 2006 *Prog. Theo. Phys.* **116** 169

[13] Fisher M E and Barber M N 1972 *Phys. Rev. Lett.* **28** 1516

[14] Landau D P 1976 *Phys. Rev.* B **14** 255

[15] Binder K 1981 *Z. Phys.* B **43** 119

[16] Peczak P, Ferrenberg A M and Landau D P 1991 *Phys. Rev.* B **43** 6087

[17] Binder K 1981 *Phys. Rev. Lett.* **47** 693

[18] Binder K and Landau D P 1984 *Phys. Rev.* B **30** 1477

[19] Challa M S S, Landau D P and Binder K 1986 *Phys. Rev.* B **34** 1841

[20] Ferrenberg A M and Swendsen R H 1988 *Phys. Rev. Lett.* **61** 2635

[21] Billoire A, Lacaze R, Morel A, Gupta S, Irbäck A and Petersson B 1990 *Phys. Rev.* B **42** 6743

[22] Rastelli E, Regina S and Tassi A 2005 *Phys. Rev.* B **71** 174406

[23] Bunker A, Gaulin B D and Kallin C 1993 *Phys. Rev.* B **48** 15861

[24] Ferrenberg A M and Landau D P 1991 *Phys. Rev.* B **44** 5081

[25] Chen K, Ferrenberg A M and Landau D P 1993 *Phys. Rev.* B **48** 3249

[26] Binder K and Rauch H 1969 *Z. Phys.* **219** 201

[27] Fisher M E 1967 *Rep. Prog. Phys.* **30** 615

[28] Mon K K 1993 *Phys. Rev.* B **47** 5497