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# Probability-changing cluster algorithm for two-dimensional *XY* and clock models

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We extend the newly proposed probability-changing cluster (PCC) Monte Carlo algorithm to the study of systems with the vector order parameter. Wolff's idea of the embedded cluster formalism is used for assigning clusters. The Kosterlitz-Thouless (KT) transitions for the two-dimensional (2D) $XY$ and $q$-state clock models are studied by using the PCC algorithm. Combined with the finite-size scaling analysis based on the KT form of the correlation length, $\xi \propto \exp(c/\sqrt{T/T_{\mathrm{KT}}-1})$, we determine the KT transition temperature and the decay exponent $\eta$ as $T_{\mathrm{KT}}=0.8933(6)$ and $\eta=0.243(4)$ for the 2D $XY$ model. We investigate two transitions of the KT type for the 2D $q$-state clock models with $q=6,8,12$ and confirm the prediction of $\eta=4/q^2$ at $T_1$, the low-temperature critical point between the ordered and $XY$-like phases, systematically.

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## I. INTRODUCTION

The two-dimensional (2D) $XY$ model shows a unique phase transition, the Kosterlitz-Thouless (KT) transition.[1,2] It does not have true long-range order, but the correlation function decays as a power of the distance at all the temperatures below the KT transition point. José *et al.*[3] studied the effect of the $q$-fold symmetry-breaking fields on the 2D $XY$ model; this is essentially the same as treating the $q$-state clock model, where only discrete values are allowed for the angle $\theta_i$ of the $XY$ spins such that

$$\theta_i = 2\pi p_i/q \quad \text{with} \quad p_i = 0,1,2,\dots,q-1. \tag{1}$$

In the limit $q\to\infty$ we get the $XY$ model. It was shown that the 2D $q$-state clock model has two phase transitions of the KT type at $T_1$ and $T_2$ ($T_1<T_2$) for $q>4$. There is an intermediate $XY$-like phase between a low-temperature ordered phase ($T<T_1$) and a high-temperature disordered phase ($T>T_2$). It was predicted that the decay critical exponent $\eta$ varies from $\eta=1/4$ at $T_2$ to $\eta=4/q^2$ at $T_1$.

Most of the above theoretical analyses relied on the renormalization group argument, and they are not exact. There have been extensive numerical studies of the 2D classical $XY$ model.[4–10] In contrast, only a limited number of numerical works have been reported on the $q$-state clock model,[11,12] and the accuracy was not good enough especially for the low-temperature phase transition. There have been no systematic studies to check the prediction of $\eta(T_1)=4/q^2$.

In numerical studies, efficient algorithms are important for getting the necessary information. The cluster update algorithms of the Monte Carlo simulation[13,14] are examples of such efforts, and they are useful for overcoming the problems of slow dynamics. Recently we proposed an effective cluster algorithm, which is called the probability-changing cluster (PCC) algorithm, of tuning the critical point automatically.[15] It is an extension of the Swendsen-Wang algorithm,[13] but we change the probability of a cluster update (essentially, the temperature) depending on the observation whether clusters are percolating or not percolating. We showed the effectiveness of the PCC algorithm for the Potts models,[15] determining the critical point and critical exponents for the second-order phase transition precisely with less numerical effort. The PCC algorithm was also applied to the 2D site-diluted Ising model, where the crossover and the self-averaging properties were studied.[16] The advantage of using the PCC algorithm in the study of random systems is as follows: The sample-dependent $T_c(L)$ for the finite system with linear size $L$ is important for taking the sample average, and the PCC algorithm is suitable for getting the sample-dependent $T_c(L)$.

There are a lot of interesting questions about the extension of the PCC algorithm. (i) Can the PCC algorithm be used for the problem of the vector order parameter, such as the $XY$ model? (ii) Can it be applied to an analysis of a transition of the KT type? (iii) Can it work even if the system shows two or more phase transitions?

The purpose of the present paper is to answer these questions. We extend the PCC algorithm so as to treat systems with the vector order parameter. The rest of the paper is organized as follows. In Sec. II, we formulate the extension of the PCC algorithm for the vector order parameter. In Sec. III, the KT transition of the 2D $XY$ model is studied with the finite-size scaling (FSS) analysis based on the KT form of the correlation length. In Sec. IV, we study the KT transitions of the 2D clock models. We investigate both phase transitions at $T_1$ and $T_2$ for the $q=6,8,12$ clock models. The summary and discussions are given in Sec. V.

## II. PCC ALGORITHM FOR VECTOR ORDER PARAMETER

Our Hamiltonian is given by

$$\mathcal{H} = -J\sum_{\langle i,j\rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_j, \tag{2}$$

where $\boldsymbol{S}_i$ is a planar unit vector $(\cos\theta_i, \sin\theta_i)$ at site $i$; $\theta_i$ takes the value of $[0,2\pi)$ for the $XY$ model and the value given in Eq. (1) for the $q$-state clock model. The summation is taken over the nearest-neighbor pairs $\langle i,j\rangle$.

In order to extend the PCC algorithm to systems with the vector order parameter, we use Wolff's idea of the embedded cluster formalism.[14] We project the vector $\boldsymbol{S}_i$ onto a randomly chosen unit vector $\boldsymbol{e}_1$ and another unit vector $\boldsymbol{e}_2$, perpendicular to $\boldsymbol{e}_1$, as

$$\boldsymbol{S}_i = \boldsymbol{e}_1 \cos\phi_i + \boldsymbol{e}_2 \sin\phi_i, \tag{3}$$

where $\phi_i$ is the angle measured from the axis of the vector $\boldsymbol{e}_1$. Then, the Hamiltonian, Eq. (2), is rewritten as

$$\mathcal{H} = -\sum_{\langle i,j\rangle} (J_{ij}^{(1)}\epsilon_i^{(1)}\epsilon_j^{(1)} + J_{ij}^{(2)}\epsilon_i^{(2)}\epsilon_j^{(2)}), \tag{4}$$

with positive effective couplings

$$J_{ij}^{(1)} = J|\cos\phi_i||\cos\phi_j|, \quad J_{ij}^{(2)} = J|\sin\phi_i||\sin\phi_j| \tag{5}$$

for two sets of Ising variables $\{\epsilon_i^{(1)}\}$ and $\{\epsilon_i^{(2)}\}$. Formally, we can restrict ourselves to the region $[0,\pi/2)$ for $\{\phi_i\}$, and we write the partition function as

$$Z = \int_0^{\pi/2}\{d\phi_i\} \sum_{\{\epsilon_i^{(1)}=\pm 1\}} \exp\left(\beta\sum_{\langle i,j\rangle} J_{ij}^{(1)}\epsilon_i^{(1)}\epsilon_j^{(1)}\right) \times \sum_{\{\epsilon_i^{(2)}=\pm 1\}} \exp\left(\beta\sum_{\langle i,j\rangle} J_{ij}^{(2)}\epsilon_i^{(2)}\epsilon_j^{(2)}\right), \tag{6}$$

with $\beta = 1/k_B T$. Then, we can use the Kasteleyn-Fortuin (KF) cluster representation for the Ising spins.[17] To make the KF cluster, we connect the bonds of parallel Ising spins with probability

$$p_{ij}^{(1,2)} = 1 - \exp(-2\beta J_{ij}^{(1,2)}). \tag{7}$$

In the PCC algorithm,[15] the cluster representation of the Ising model is used in two ways. First, we flip all the spins on any KF cluster to one of two states, that is, $+1$ or $-1$, as in the Swendsen-Wang algorithm.[13] Second, we change the KF probability, Eq. (7), depending on the observation whether clusters are percolating or not. It is based on the fact that the spin-spin correlation function $G(\boldsymbol{r}_i - \boldsymbol{r}_j)$ becomes nonzero for $|\boldsymbol{r}_i - \boldsymbol{r}_j| \to \infty$ at the same point as the percolation threshold. For the $XY$ model in the embedded cluster formalism, the spin-spin correlation function is written as

$$\begin{aligned} G(\boldsymbol{r}_i - \boldsymbol{r}_j) &= \langle \boldsymbol{S}_i \cdot \boldsymbol{S}_j \rangle = \langle |\cos\phi_i|\,|\cos\phi_j|\,\epsilon_i^{(1)}\epsilon_j^{(1)}\rangle \\ &\quad + \langle |\sin\phi_i|\,|\sin\phi_j|\,\epsilon_i^{(2)}\epsilon_j^{(2)}\rangle \\ &= \langle A_{ij}\Theta^{(1)}(\boldsymbol{r}_i,\boldsymbol{r}_j)\rangle + \langle B_{ij}\Theta^{(2)}(\boldsymbol{r}_i,\boldsymbol{r}_j)\rangle, \end{aligned} \tag{8}$$

where $\langle \cdots \rangle$ represents the thermal average. The function $\Theta(\boldsymbol{r}_i,\boldsymbol{r}_j)$ is equal to 1 (0) if the sites $i$ and $j$ belong to the same (different) cluster, and $A_{ij}$ and $B_{ij}$ are some constants. Thus, the system is regarded as percolating if $\epsilon^{(1)}$ or $\epsilon^{(2)}$ Ising spins are percolating. When treating the cluster spin update, one may consider Ising spins of a single type projected onto a randomly chosen axis, as in the original Wolff's proposal.[14] However, we should consider Ising spins of both types perpendicular to each other for checking the percolation.

The procedure of Monte Carlo spin update is as follows: (i) Start from some spin configuration and some value of $\beta$. (ii) Choose a unit vector $\boldsymbol{e}_1$ randomly. (iii) Construct the KF clusters for $\epsilon^{(1)}$ and $\epsilon^{(2)}$ using the probability, Eq. (7), and check whether the system is percolating or not. Flip all the spins on any KF cluster to $+1$ or $-1$ for both $\epsilon^{(1)}$ and $\epsilon^{(2)}$ Ising spins. (iv) If the system is percolating (not percolating), decrease (increase) $\beta$ by $\Delta\beta$ $(>0)$. (v) Go back to the process (ii).

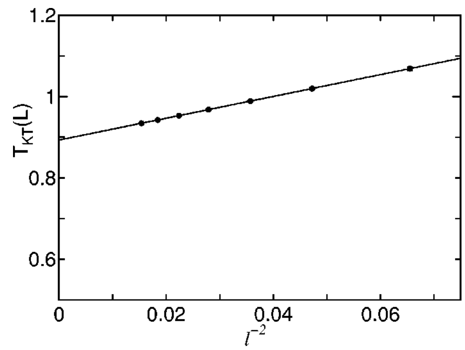


FIG. 1. Plot of $T_{\mathrm{KT}}(L)$ of the 2D $XY$ model for $L=8$, 16, 32, 64, 128, 256, and 512, where $l=\ln bL$.

As $\Delta\beta$ becomes small, the distribution of $\beta$ becomes a sharp Gaussian distribution around the mean value $\beta_c(L)$, which depends on the system size $L$. We approach the canonical ensemble in this limit, and the existence probability $E_p$, the probability that the system percolates, becomes 1/2 at $\beta_c(L)$.

## III. *XY* MODEL

We have made simulations for the classical $XY$ model on a square lattice with system sizes $L=8$, 16, 32, 64, 128, 256, and 512. After 20 000 Monte Carlo sweeps of determining $\beta_c(L)$ with gradually reducing $\Delta\beta$, we have made 10 000 Monte Carlo sweeps to take the thermal average; we have made 100 runs for each size to get better statistics and to evaluate the statistical errors. As for the criterion to determine percolating, we have employed the topological rule[15,18] in the present study. The topological rule is that some cluster winds around the system in at least one of the $D$ directions in $D$-dimensional systems.

Let us start with the size dependence of the transition temperature. We use the FSS analysis based on the KT form of the correlation length,

$$\xi \propto \exp(c/\sqrt{t}), \tag{9}$$

with $t=(T-T_{\mathrm{KT}})/T_{\mathrm{KT}}$. Using the PCC algorithm, we locate the temperature $T_{\mathrm{KT}}(L) = 1/k_B\beta_c(L)$, the existence probability $E_p$ of which is 1/2. Then, using the FSS form of $E_p$, that is, $E_p = E_p(\xi/L)$, we have the relation

$$T_{\mathrm{KT}}(L) = T_{\mathrm{KT}} + \frac{c^2 T_{\mathrm{KT}}}{(\ln bL)^2}. \tag{10}$$

We plot $T_{\mathrm{KT}}(L)$ as a function of $l^{-2}$ with $l=\ln bL$ for the best-fitted parameters in Fig. 1. We represent the temperature in units of $J/k_B$. The error bars are smaller than the size of the marks. Our estimate of $T_{\mathrm{KT}}$ is 0.8933(6); the number in

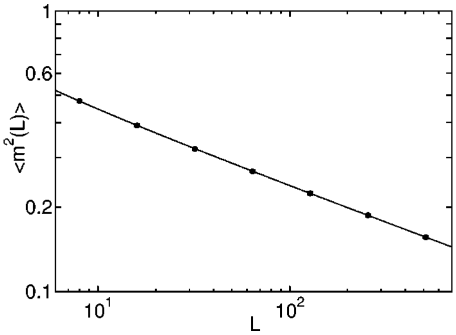


FIG. 2. Logarithmic plot of $\langle m^2(L)\rangle$ at $T_{\mathrm{KT}}(L)$ of the 2D $XY$ model for $L=8$, 16, 32, 64, 128, 256, and 512.

the parentheses denotes the uncertainty in the last digits. We have estimated the uncertainty by the $\chi^2$ test of the data for 100 samples. This value is consistent with the estimates of recent studies: 0.892 13(10) by Monte Carlo simulation[8] and 0.894 by short-time dynamics.[9] The constant $c$, in Eq. (10), is estimated as $c=1.73(2)$.

Let us consider the magnetization $\langle m^2(L)\rangle$ at $T_{\mathrm{KT}}(L)$ to discuss the critical exponent $\eta$. In Fig. 2, we plot $\langle m^2(L)\rangle$ as a function of $L$ in a logarithmic scale. We expect a FSS of the form $\langle m^2(L)\rangle \propto L^{-\eta}$, but there are small corrections. The importance of the multiplicative logarithmic corrections were pointed out.[2,19] Using the form

$$\langle m^2(L)\rangle = AL^{-\eta}(\ln b'L)^{-2r}, \tag{11}$$

we obtain $\eta=0.243(4)$ and $r=0.038(5)$. We show the fitting curve obtained by using Eq. (11) in Fig. 2. This value of $\eta$ is a little bit smaller than the theoretical prediction, 1/4 $(=0.25)$. Our logarithmic-correction exponent $r$ is compatible with Janke's result $r=0.0560(17)$ for thermodynamic data,[19] but different from the theoretical prediction $r=-1/16$.[2]

## IV. CLOCK MODEL

Next turn to the $q$-state clock model. Because of the reflection symmetry, we confine ourselves to the case of even $q$. Then, the same procedure can be used as the $XY$ model. One thing we should have in mind is that the axis of the vector $\boldsymbol{e}_1$ should be chosen from one of $q$ directions in Eq. (1) or the middle of two of them. We plot the high-temperature transition temperature $T_2(L)$ of the six-state clock model as a function of $l^{-2}$ in Fig. 3. The estimate of $T_2$ is 0.9008(6), which is more precise than the previous estimates: 0.92(1) (Ref. 11) and 0.90 (Ref. 12). The plot of $\langle m^2(L)\rangle$ at $T_2(L)$ as a function of $L$ for the six-state clock model is given in Fig. 4. The estimate of $\eta$ is 0.243(4) by the analysis of the multiplicative logarithmic corrections, Eq. (11), and the exponent $r$ is estimated as 0.037(5).

For the second-order transition, the curves of the existence probability $E_p$ of different sizes cross at $T_c$ as far as the corrections to FSS are negligible; this is the same as the behavior of the Binder ratio.[20] For the KT transition, however, $T_{\mathrm{KT}}$ is not the crossing point but the spray-out point. Therefore, $T_2$ can be searched only from the high-temperature side and $T_1$ only from the low-temperature side. The value of $E_p$ at $T_1$ is close to 1. In principle, we can use the same procedure as the study of $T_2$; we may change the setting value of $E_p$, 1/2, to a higher one by introducing a biased random walk. However, it is difficult to resolve the size dependence for lower temperatures. Therefore, we employ a slightly different approach for an analysis of the phase transition at $T_1$. When judging whether clusters are percolating or not, we consider another type of clusters. Instead of choosing the vector $\boldsymbol{e}_1$ randomly in Eq. (3), we choose the vector $\boldsymbol{e}_1$ as

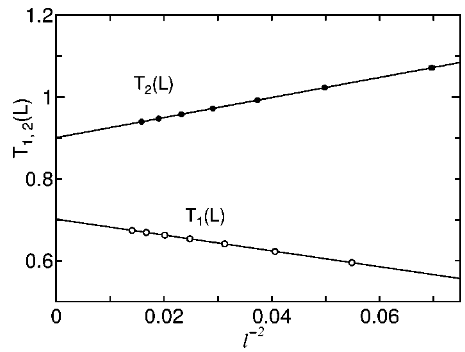


FIG. 3. Plots of $T_1(L)$ and $T_2(L)$ of the 2D six-state clock model for $L=8$, 16, 32, 64, 128, 256, and 512, where $l=\ln bL$.

$$\boldsymbol{M}=|\boldsymbol{M}|\boldsymbol{e}_1, \tag{12}$$

with $\boldsymbol{M}=\Sigma_i \boldsymbol{S}_i$, or more generally we may choose $\boldsymbol{e}_1$ such that

$$\boldsymbol{M}=|\boldsymbol{M}|(\boldsymbol{e}_1\cos\phi+\boldsymbol{e}_2\sin\phi), \tag{13}$$

with some fixed angle $\phi$. With this choice, the existence probability for the percolation of only $\epsilon^{(1)}$ (or $\epsilon^{(2)}$) Ising spins holds the same FSS property as the total $E_p$. As a result, we can control the value of $E_p^{(1)}$ at $T_1$ so as to apply the FSS analysis easily with an appropriate $\phi$.

The low-temperature transition temperature $T_1(L)$ of the six-state clock model obtained by the above modified approach is plotted as a function of $l^{-2}$ also in Fig. 3. As the angle $\phi$ in Eq. (13), we have used $\pi/3$. Our estimate of $T_1$ is 0.7014(11), which is more precise again than the previous estimates: 0.68(2) (Ref. 11) and 0.75 (Ref. 12). The plot of $\langle m^2(L)\rangle$ at $T_1(L)$ for the six-state clock model is also given

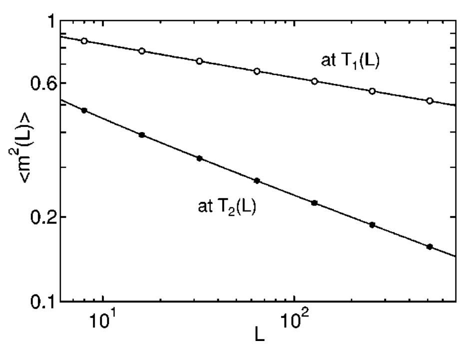


FIG. 4. Logarithmic plots of $\langle m^2(L)\rangle$ at $T_1(L)$ and $T_2(L)$ of the 2D six-state clock model for $L=8$, 16, 32, 64, 128, 256, and 512.

TABLE I. Transition temperatures and exponents $\eta$ for the 2D $q$-state clock model.

| | $T_2$ | $\eta(T_2)$ | $T_1$ | $\eta(T_1)$ |
|---|---|---|---|---|
| $q=6$ | 0.9008(6) | 0.243(4) | 0.7014(11) | 0.113(3) |
| $q=8$ | 0.8936(7) | 0.243(4) | 0.4259(4) | 0.0657(2) |
| $q=12$ | 0.8937(7) | 0.246(5) | 0.1978(5) | 0.0270(5) |
| $XY(q=\infty)$ | 0.8933(6) | 0.243(4) | ——— | ——— |

in Fig. 4. The estimate of $\eta$ is 0.113(3) by the analysis of the multiplicative logarithmic corrections, Eq. (11), and the exponent $r$ is estimated as 0.017(4). The previous estimates of $\eta$ are 0.100 (Ref. 11) and 0.15 (Ref. 12).

We have also made simulations for $q=8$ and $q=12$. The estimates of the transition temperatures $T_1, T_2$ and those of $\eta(T_1)$ and $\eta(T_2)$ for $q=6$, 8, 12, and $\infty$ (the $XY$ model) are tabulated in Table I. The $1/q^2$ dependence of the transition temperatures and exponents are shown in Fig. 5. There, the exact results for $q=4$ are also given: that is, the Ising singularity at $T_c=[\ln(\sqrt{2}+1)]^{-1}=1.1346$ with $\eta=1/4$. The transition temperature $T_1$ becomes smoothly lower with larger $q$; in the lowest order we find that $T_1 \propto 1/q^2$, which is consistent with the theoretical prediction.[3] The critical exponent $\eta$ at $T_2$ is a universal constant and compatible with the theoretical prediction $\eta=1/4$. The estimates of the critical exponent $\eta$ at $T_1$ remarkably coincide with the theoretical prediction $\eta=4/q^2$: $1/9=0.111$ for $q=6$, $1/16=0.0625$ for $q=8$, and $1/36=0.0278$ for $q=12$.

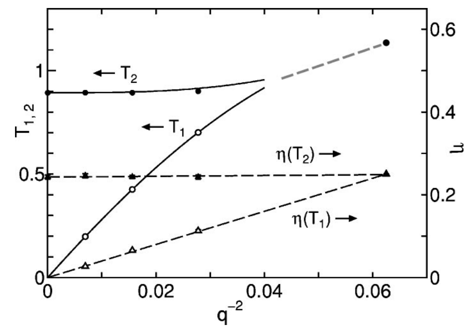


FIG. 5. Transition temperatures and critical exponents as a function of $1/q^2$ for the 2D $q$-state clock model.

## V. SUMMARY AND DISCUSSIONS

To summarize, we have extended the PCC algorithm[15] to the study of the $XY$ and clock models. Wolff's idea of the embedded cluster formalism[14] is used for treating the system with the vector order parameter. The KT transitions of the 2D $XY$ and clock models are studied by using a FSS analysis based on the KT form of the correlation length. For dealing with the low-temperature transition temperature $T_1$, we have employed a slightly modified algorithm. Investigating the $q=6,8,12$ clock models, we have systematically confirmed the prediction of $\eta(T_1)=4/q^2$. We have shown that small logarithmic corrections are present in the KT transitions. The sign of the logarithmic-correction exponent $r$ is positive for all cases of the $XY$ model and the clock models at both $T_1$ and $T_2$, which is compatible with Janke's result,[19] but different from the theoretical prediction that $r$ is negative.[2] The present precise numerical results may stimulate the refined renormalization-group study of the KT transitions.

In the previous numerical studies of the KT transitions, one might resort to a big scale calculation using an extensive computer resource,[5] or one might use some special boundary conditions.[8] It is due to the subtlety of the KT phase transitions; that is, $T_{\mathrm{KT}}$ is not the crossing point but the spray-out point of the existence probability or the Binder parameter. Moreover, the low-temperature transition $T_1$ for the clock model is difficult to study because the system is nearly ordered; it is more difficult for larger $q$. We should stress that using the present efficient method of numerical simulation, we have successfully made a systematic study of the $XY$ and clock models with much less effort.

Our formalism of the vector order parameter is easily extended to the general $O(n)$ model, where percolation of $n$ types of Ising spins will be considered. Then, more problems of interest can be studied by the PCC algorithm. The PCC algorithm can be also applied to the quantum Monte Carlo simulation with the cluster algorithm.[21,22] It will be interesting to compare the present result with the quantum $XY$ model.

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[1] J. Kosterlitz and D. Thouless, J. Phys. C **6**, 1181 (1973). See also V. L. Berezinskii, Zh. Éksp. Teor. Fiz. **59**, 907 (1970) [Sov. Phys. JETP **32**, 493 (1971)].
[2] J. M. Kosterlitz, J. Phys. C **7**, 1046 (1974).
[3] J. V. José, L. P. Kadanoff, S. Kirkpatrick, and D. R. Nelson, Phys. Rev. B **16**, 1217 (1977).
[4] H. Weber and P. Minnhagen, Phys. Rev. B **37**, 5986 (1988).
[5] R. Gupta and C. F. Baillie, Phys. Rev. B **45**, 2883 (1992).
[6] H. Kawamura and M. Kikuchi, Phys. Rev. B **47**, 1134 (1993).
[7] P. Butera and M. Comi, Phys. Rev. B **47**, 11 969 (1993).
[8] P. Olsson, Phys. Rev. B **52**, 4526 (1995).
[9] B. Zheng, M. Schulz, and S. Trimper, Phys. Rev. E **59**, R1351 (1999).
[10] S. G. Chung, Phys. Rev. B **60**, 11 761 (1999).
[11] M. S. S. Challa and D. P. Landau, Phys. Rev. B **33**, 437 (1986).
[12] A. Yamagata and I. Ono, J. Phys. A **24**, 265 (1991).

[13] R. H. Swendsen and J. S. Wang, Phys. Rev. Lett. **58**, 86 (1987).
[14] U. Wolff, Phys. Rev. Lett. **62**, 361 (1989).
[15] Y. Tomita and Y. Okabe, Phys. Rev. Lett. **86**, 572 (2001).
[16] Y. Tomita and Y. Okabe, Phys. Rev. E **64**, 036114 (2001).
[17] P. W. Kasteleyn and C. M. Fortuin, J. Phys. Soc. Jpn., Suppl. **26**, 11 (1969); C. M. Fortuin and P. W. Kasteleyn, Physica (Amsterdam) **57**, 536 (1972).
[18] J. Machta, Y. S. Choi, A. Lucke, T. Schweizer, and L. V. Chayes, Phys. Rev. Lett. **75**, 2792 (1995).
[19] W. Janke, Phys. Rev. B **55**, 3580 (1997).
[20] K. Binder, Z. Phys. B: Condens. Matter **43**, 119 (1981).
[21] H. G. Evertz, G. Lana, and M. Marcu, Phys. Rev. Lett. **70**, 875 (1993).
[22] N. Kawashima and J. E. Gubernatis, Phys. Rev. Lett. **73**, 1295 (1994).