Cluster analysis and finite-size scaling for Ising spin systems

Yusuke Tomita and Yutaka Okabe[*]
Department of Physics, Tokyo Metropolitan University, Hachioji, Tokyo 192-0397, Japan

Chin-Kun Hu[†]
Institute of Physics, Academia Sinica, Nankang, Taipei 11529, Taiwan
(Received 25 November 1998; revised manuscript received 10 May 1999)

Based on the connection between the Ising model and a correlated percolation model, we calculate the distribution function for the fraction (c) of lattice sites in percolating clusters in subgraphs with n percolating clusters, $f_n(c)$, and the distribution function for magnetization (m) in subgraphs with n percolating clusters, $p_n(m)$. We find that $f_n(c)$ and $p_n(m)$ have very good finite-size scaling behavior and that they have universal finite-size scaling functions for the model on square, plane triangular, and honeycomb lattices when aspect ratios of these lattices have the proportions $1:\sqrt{3}/2:\sqrt{3}$. The complex structure of the magnetization distribution function $p(m)$ for the system with large aspect ratio could be understood from the independent orientations of two or more percolation clusters in such a system. [S1063-651X(99)09609-9]

PACS number(s): 05.50.+q, 64.60.Ak, 75.10.-b

Universality and scaling are two important concepts in the modern era of critical phenomena [1] and, for analyzing the simulation or experimental data of finite critical systems, one often appeals to finite-size scaling [2–4] where both critical exponents and finite-size scaling functions play an important role. The universality of critical exponents has been well known for a long time [1], but the universality of finite-size scaling functions received much attention only in recent years [5–10]. In 1984, Privman and Fisher first proposed the idea of universal finite-size scaling functions (UFSSF's) with nonuniversal metric factors [3]. In 1995 and 1996, Hu, Lin, and Chen (HLC) [5] applied a histogram Monte Carlo simulation method [11] to calculate the existence probability [11] (also called the crossing probability [12]) E_p, the percolation probability P, the probability for the appearance of n percolating clusters W_n [5] of site and bond percolation on finite square (sq), plane triangular (pt), and honeycomb (hc) lattices, whose aspect ratios approximately have the relative proportions $1:\sqrt{3}/2:\sqrt{3}$ considered by Langlands *et al.* [12]. Using nonuniversal metric factors, HLC found that the six percolation models have very nice UFSSF's for E_p, P, and W_n near the critical points [5] and, at the critical point, the average number of percolating clusters increases linearly with aspect ratios of the lattices [5]. Using the Monte Carlo simulation, Okabe and Kikuchi found UFSSF's for the Binder parameter g [13] and magnetization distribution functions $p(m)$ of the Ising model on planar lattices [6], and Wang and Hu found UFSSF's for dynamic critical phenomena of the Ising model [7]. Based on the connection between the q-state bond correlated percolation model (BCPM) and the q-state Potts model [14] Hu, Chen, and Lin found UFSSF's for E_p and W_n of the q-state BCPM without using nonuniversal metric factors [9]. It is of interest to gain a deeper understanding of the UFSSF's for W_n and P for the system with multiple percolating clusters.

In this paper, based on the connection between the Ising model, i.e., the two-state Potts model and the two-state BCPM, we use the Monte Carlo method to calculate the distribution function for the fraction (c) of lattice sites in percolating clusters in subgraphs with n percolating clusters, $f_n(c)$, and the distribution function for magnetization (m) in subgraphs with n percolating clusters, $p_n(m)$. We find that $f_n(c)$ and $p_n(m)$ have very good finite-size scaling behavior and that they have UFSSF's for the model on sq, pt, and hc lattices when aspect ratios of these lattices have the proportions $1:\sqrt{3}/2:\sqrt{3}$. Since W_n and P of the two-state BCPM for the Ising model may be calculated from $f_n(c)$, the universality of finite-size scaling functions for W_n and P are related to the universality of finite-size scaling functions for $f_n(c)$. The complex structure of $p(m)$ for the system with a large aspect ratio could be understood from the independent orientations of two or more percolation clusters in such a system. Our work suggests many problems for further research.

The Hamiltonian of the Ising model on an $L_1 \times L_2$ lattice G of N_b bonds is given by $\mathcal{H} = -J\Sigma_{\langle i,j \rangle} \sigma_i \sigma_j - h\Sigma_i \sigma_i$, where $\sigma_i = \pm 1$, $J > 0$ and is the ferromagnetic coupling constant between the nearest-neighbor Ising spins, and h is the external magnetic field. Using subgraph expansion, Hu [14] showed that the partition function of the Ising model on G may be written as

$$Z_N = e^{KN_b} \sum_{G' \subseteq G} p^{b(G')}(1-p)^{N_b - b(G')}$$

$$\times \prod_{\text{cluster}} [2\cosh(Bn_c(G'))], \qquad (1)$$

where $p = 1 - e^{-2K}$, $K = J/(k_B T)$, $B = h/(k_B T)$, $b(G')$ is the number of occupied bonds in G', and the sum is over all subgraphs G' of G; the product extends over all clusters in a given G' and $n_c(G')$ is the number of sites in each cluster. When $B = 0$, Eq. (1) reduces to the result of Ref. [15]. The sites connected by occupied bonds are in the same cluster; all spins in a cluster must be in the same direction, which may

*Electronic address: okabe@phys.metro-u.ac.jp
†Electronic address: huck@phys.sinica.edu.tw

be up or down. Using Z_N of Eq. (1), Hu found that the spontaneous magnetization and the magnetic susceptibility of the Ising model are related to the percolation probability P and the mean cluster size of the (two-state) BCPM, such that the probability weight for the appearance of a subgraph G' of $b(G')$ bonds and $n(G')$ clusters is given by $\pi(G',p) = p^{b(G')}(1-p)^{N_b - b(G')}2^{n(G')}$. Such a connection ensures that the phase transition of the Ising model is the percolation transition of the BCPM. The extension of the probability weight $\pi(G',p)$ to a q-state Potts model is simply achieved by replacing 2 with q in $\pi(G',p)$. From $\pi(G',p)$ we can define

$$E_p(G,p) = \sum_{G'_p \subseteq G} \pi(G'_p,p) / \sum_{G' \subseteq G} \pi(G',p), \qquad (2)$$

which is called the existence probability of the BCPM. Here the sum in the denominator is over all subgraphs G' of G and the sum in the numerator is restricted to all percolating subgraphs G'_p of G. In Ref. [16], Hu and Chen found that $E_p(G,p)$ has very good finite-size scaling behavior. In Ref. [9], Hu, Chen, and Lin found that $E_p(G,p)$ has a UFSSF.

In the present paper we use the Wolff algorithm [17] for spin update and study the percolating properties of clusters on planar lattices with periodic boundary conditions for both directions. For the assignment of a bond-percolating cluster, we consider free and periodic boundary conditions in the

vertical and horizontal directions, respectively; that is, a cluster that extends from the top row to the bottom row is a percolating cluster.

We first consider the fraction of lattice sites in the percolating clusters, c, and denote the probability distribution function of c by $f(c)$. The average value of c gives the percolation probability P,

$$\langle c \rangle = \int_0^1 c f(c) dc = P, \qquad (3)$$

and plays the role of order parameter in the percolation problem. To study c in subgraphs with exactly n percolating clusters, we decompose $f(c)$ by the number of percolating clusters, n; that is,

$$f(c) = \sum_{n=1}^{\infty} f_n(c). \qquad (4)$$

We should note that

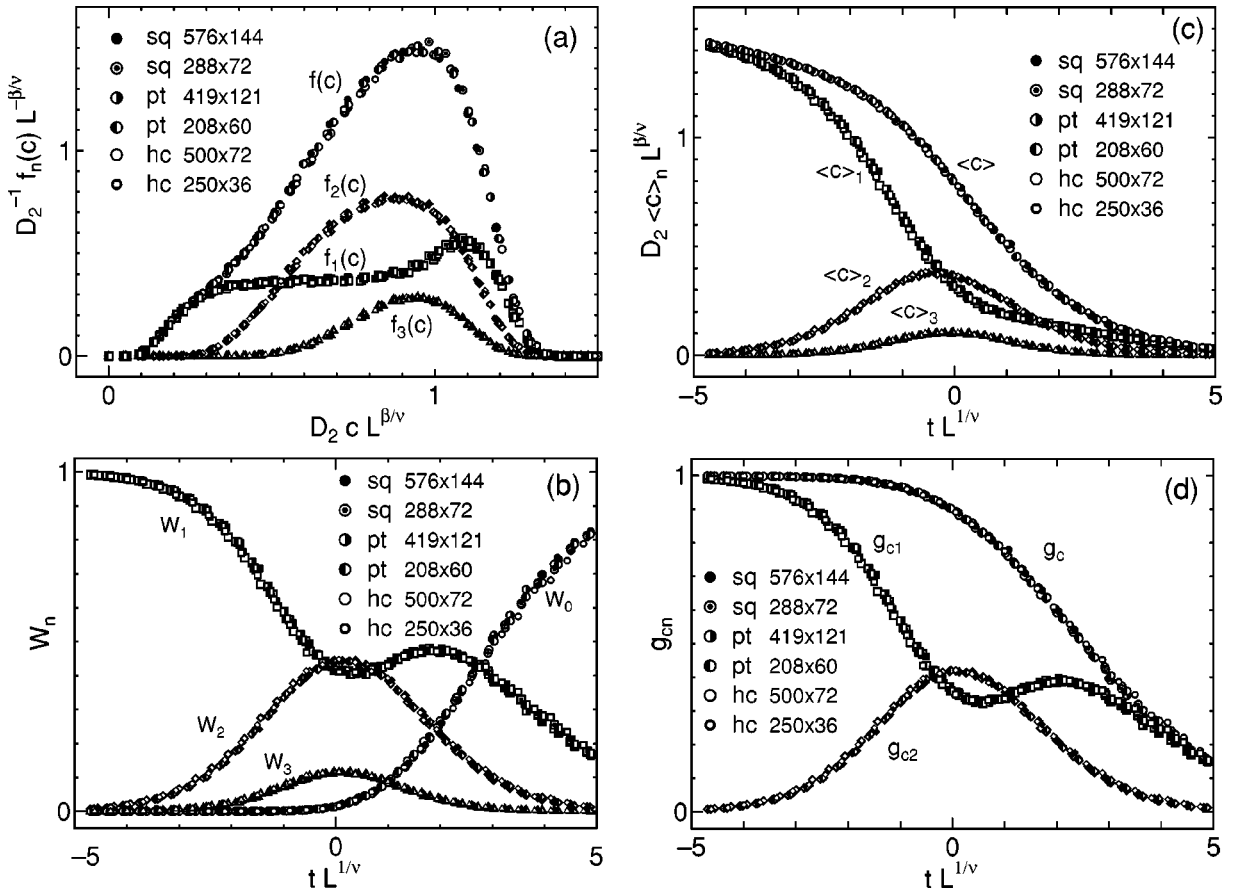$$\int_0^1 f_n(c) dc = W_n, \qquad (n = 1, \ldots, \infty) \qquad (5)$$

and

FIG. 1. Universal finite-size scaling functions for the Ising clusters on the sq, pt, and hc lattices. (a) $D_2^{-1} f_n(c)L^{-\beta/\nu}$ and $D_2^{-1} f(c)L^{-\beta/\nu}$ at the critical point as a function of $D_2 c L^{\beta/\nu}$; (b) W_n as a function of $tL^{1/\nu}$; (c) $D_2 \langle c \rangle_n L^{\beta/\nu}$ and $D_2 \langle c \rangle L^{\beta/\nu}$ as a function of $tL^{1/\nu}$; and (d) $g_{cn}(=\langle c \rangle_n^2/\langle c^2 \rangle_n)$ and $g_c(=\langle c \rangle^2/\langle c^2 \rangle)$ as a function of $tL^{1/\nu}$.

$$\sum_{n=1}^{\infty} W_n = 1 - W_0 = E_p(G,p). \tag{6}$$

We may consider the quantity,

$$\langle c \rangle_n = \int_0^1 c f_n(c) dc, \quad (n=1,\ldots,\infty), \tag{7}$$

which is the fraction of lattice sites in the n percolating clusters. In other words, we decompose $\langle c \rangle$ by the number of percolating clusters, such that

$$\langle c \rangle = \sum_{n=1}^{\infty} \langle c \rangle_n = P. \tag{8}$$

The probability distribution of the magnetization, $p(m)$, is an important quantity in the phase transition problem [6,10]. Let us decompose $p(m)$ by the number of percolating clusters in the same way as in $f(c)$,

$$p(m) = \sum_{n=0}^{\infty} p_n(m). \tag{9}$$

Now we have the relation

$$\int_{-1}^1 p_n(m) dm = W_n, \quad (n=0,\ldots,\infty). \tag{10}$$

It should be noted that the relation between $f_n(c)$ and $p_n(m)$ is not a simple one, especially for a system with multiple percolating clusters. There are two type of clusters, that is, the cluster with up spins and that with down spins. We may divide the fraction of lattice sites in percolating clusters, c, into two classes, c_+ and c_-. By definition, $c = c_+ + c_-$ and, to the leading order, $m \sim c_+ - c_-$. If there is only a single percolating cluster, $m \sim c_+$ or $m \sim c_-$; thus, $m^2 \sim c^2$ in the leading contribution. However, if there are two or more percolating clusters, the relation is not trivial, and this is the origin of the complex structure of $p(m)$ for the lattices with large aspect ratio a. Therefore, the study of c and m becomes more interesting in the case of multiple percolating clusters.

According to the theory of finite-size scaling [2], if a quantity Q has a singularity of the form $Q(t) \sim t^{\omega}$ near the criticality $t=0$, then the corresponding quantity $Q(L,t)$ for the finite system with the linear size L has a scaling form $Q(L,t) \sim L^{-\omega/\nu} X(tL^{1/\nu})$, where ν is the correlation-length exponent and is 1 for the two-dimensional (2D) Ising model. The finite-size scaling is also applicable to the distribution function of Q. At the criticality $t=0$, we have a finite-size scaling form $p(Q;L,t=0) \sim L^{\omega/\nu} Y(QL^{\omega/\nu})$. Thus, we expect the following finite-size scaling relations: $W_n(t) \sim X_n^a(tL^{1/\nu})$, $\langle c \rangle_n(t) \sim L^{-\beta/\nu} X_n^b(tL^{1/\nu})$, $f_n(c;t=0) \sim L^{\beta/\nu} Y_n^a(cL^{\beta/\nu})$, and $p_n(m;t=0) \sim L^{\beta/\nu} Y_n^b(mL^{\beta/\nu})$, where β is the order-parameter exponent and is 1/8 for the 2D Ising model.

The finite-size scaling functions usually depend on the lattice or other details of the system. However, with appropriate choices of nonuniversal metric factors D_1 and D_2,

$$D_2 Q(L,t) = L^{-\omega/\nu} \hat{X}(D_1 t L^{1/\nu}), \tag{11}$$

$$p(Q;L,t=0) = D_2 L^{\omega/\nu} \hat{Y}(D_2 Q L^{\omega/\nu}), \tag{12}$$

the finite-size scaling functions $\hat{X}, \hat{Y}$ could become universal. This concept of the UFSSF was first proposed by Privman and Fisher [3], and has been recently confirmed for the percolation problem [5,8] and the Ising model [6,9]. We should note that the UFSSF's still depend on boundary conditions [5].

To study the finite-size scaling and the universality of $f_n(c)$, $f(c)$, $p_n(m)$, and $p(m)$, we calculate $f_n(c)$, $f(c)$, $p_n(m)$, $p(m)$, W_n, $\langle c \rangle_n$, $\langle c \rangle$, g_{cn}, and g_c for the BCPM on sq, pt, and hc lattices whose aspect ratios approximately have the proportions $1:\sqrt{3}/2:\sqrt{3}$ and each kind of lattice has two linear dimensions; here $g_{cn} = \langle c \rangle_n^2 / \langle c^2 \rangle_n$, $g_c = \langle c \rangle^2 / \langle c^2 \rangle$, and the second moments of c are defined as in Eqs. (7) and (3). We note that g_{cn} and g_c have the same finite-size scaling property as the Binder parameter [13].

The calculated $D_2^{-1} f_n(c) L^{-\beta/\nu}$ and $D_2^{-1} f(c) L^{-\beta/\nu}$, at the critical point as a function of $D_2 c L^{\beta/\nu}$, are shown in Fig. 1(a). The lattice sizes are given within the figure. The aspect ratio is $a=4$ for the sq lattice, and corresponding equivalent ratios for other lattices. The calculated W_n, $D_2 \langle c \rangle_n L^{\beta/\nu}$ (also $D_2 \langle c \rangle L^{\beta/\nu}$), and g_{cn} (also g_c), as a function of $tL^{1/\nu}$ $[t=(T-T_c)/T_c]$, are presented in Figs. 1(b), 1(c), and 1(d), respectively. The calculated $D_2^{-1} p_n(m) L^{-\beta/\nu}$ as a function
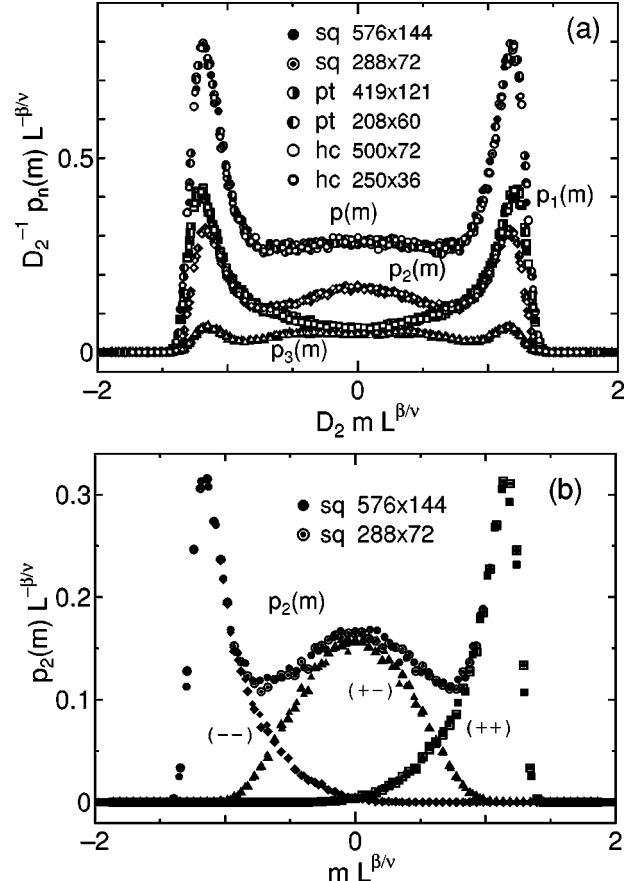

FIG. 2. (a) $D_2^{-1} p_n(m) L^{-\beta/\nu}$ at $T=T_c$ as a function of $D_2 m L^{\beta/\nu}$. (b) $p_2(m)$ at $T=T_c$ is decomposed into three classes: $p_{++}(m)$, $p_{--}(m)$, and $p_{+-}(m)$.
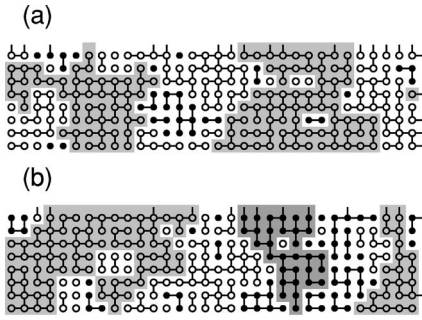
FIG. 3. Examples of snapshots of the Ising system with the aspect ratio $a=4$. Up and down spins are represented by open and closed circles, and active bonds are represented by a solid line. Percolating clusters are distinguished by the shaded areas. There are two percolating clusters with up spins in (a), whereas one percolating cluster is up and the other is down in (b).

of $D_2 m L^{\beta/\nu}$ is shown in Fig. 2(a). The metric factors D_1 and D_2 for the sq lattice are chosen as 1 [18]. The values of D_1 for the pt and hc lattices are 1.00 ± 0.01, which are consistent with the results of Ref. [9]; the values of D_2 for the pt and hc lattices are 1.02 ± 0.01 and 0.98 ± 0.01, respectively. Since we have estimated D_1 as 1.00 ± 0.01 for the pt and hc lattices, we have omitted D_1 in the horizontal axes of the figures. Figures 1(a)–1(d) and Fig. 2(a) show that the calculated quantities have very good finite-size scaling behavior and the universality is also well satisfied. We should note that the metric factors D_1 and D_2 are the same for all quantities.

Figure 2(a) shows that $p(m)$ at $T=T_c$ has a broad peak centered at $m=0$, in addition to two peaks of positive and negative m for the system with the aspect ratio $a=4$ for the sq lattice. This is in contrast to the case of $a=1$ where $p(m)$ has only two distinct peaks of positive and negative m. Such a dependence of $p(m)$ on a has already been pointed out in Ref. [10]. From Fig. 2(a), we see that the broad peak of $p(m)$ centered at $m=0$ mainly comes from $p_2(m)$. There are two types of Ising clusters, that is, the clusters with up spins or the clusters with down spins. Therefore, if there are many percolating clusters, the combination of the percolating clusters with up spins and those with down spins makes it possible for the total magnetization to become close to 0. It is known that the normalized fourth moment of m, or the Binder parameter, at the critical point depends on the aspect ratio [10,19]. The origin of such a dependence can be attributed to the structure of many percolating clusters. To clarify this situation, we decompose $p_2(m)$ at $T=T_c$ into three classes, $p_{++}(m)$, $p_{--}(m)$, and $p_{+-}(m)$, shown in Fig. 2(b). We assign three peaks in $p_2(m)$ by the contribution from $p_{++}(m)$, $p_{--}(m)$, and $p_{+-}(m)$. Examples of snapshots of the Ising system with two percolating clusters are presented in Figs. 3(a) and 3(b). In Fig. 3(a) both percolating clusters are up; in Fig. 3(b) one percolating cluster is up and another percolating cluster is down.

From W_n, we may calculate the average number of percolating clusters by $\langle n \rangle = \Sigma_n n W_n$. At the critical point, the values of W_n and $\langle n \rangle$, as a function of the aspect ratio $a = L_1/L_2$, are plotted in Figs. 4(a) and 4(b), respectively. We see that $\langle n \rangle$ increases linearly with a for large a, which is
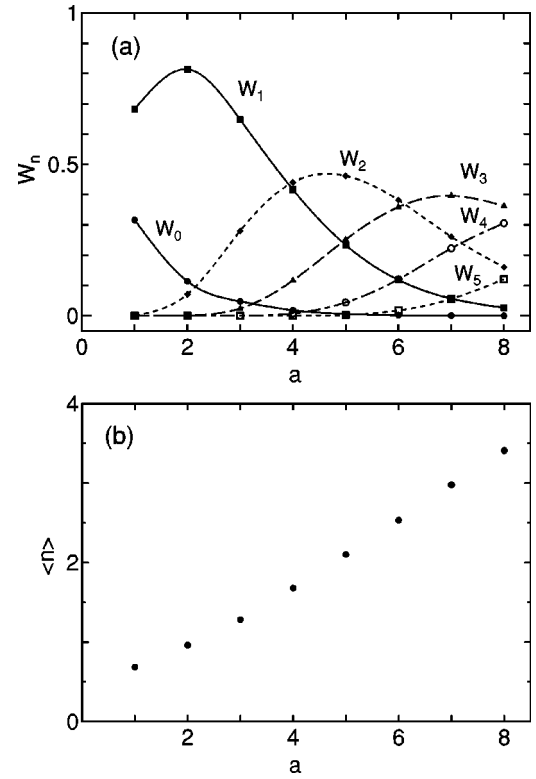

FIG. 4. (a) W_n at $T=T_c$ as a function of $a=L_1/L_2$. (b) $\langle n \rangle$ at $T=T_c$ as a function of a.

similar to the case of random percolation [5,20]. The slope of $\langle n \rangle$ versus a in Fig. 4(b) is approximately 0.5.

Following the study of W_n for random percolation by Hu and Lin [5], there have been many analytic and numerical studies of W_n in different random percolation problems [21]; it is of interest to extend such studies to the BCPM of the Ising model. On the other hand, we can extend the study of $f_n(c)$ and $\langle c \rangle_n$ to the random percolation problem. It is interesting to compare the results for the BCPM and those for the random percolation problem. We may also extend the present study to the bond-diluted or the site-diluted Ising model, which can be mapped into percolation models [22]. The critical phenomena of the percolating properties of the Ising model are governed by the Ising fixed point (for example, $\nu=1$) whereas, at the percolation threshold, the critical phenomena are governed by the random percolation fixed point ($\nu=4/3$). The crossover from the Ising fixed point to the random percolation fixed point in the process of dilution is highly interesting, especially for the properties depending on the number of the percolating clusters. The studies in these directions are in progress.

[1] H. E. Stanley, *Introduction to Phase Transitions and Critical Phenomena* (Oxford University Press, New York, 1971).

[2] M. E. Fisher, in *Critical Phenomena*, *Proceedings of the International School of Physics "Enrico Fermi,"* Course 51, Varenna, 1970, edited by M. S. Green (Academic, New York, 1971), Vol. 51, p. 1; in *Finite-size Scaling*, edited by J. L. Cardy (North-Holland, New York, 1988).

[3] V. Privman and M. E. Fisher, Phys. Rev. B **30**, 322 (1984).

[4] D. Stauffer and A. Aharony, *Introduction to Percolation Theory*, revised 2nd ed. (Taylor & Francis, London, 1994).

[5] C.-K. Hu, C.-Y. Lin, and J.-A. Chen, Phys. Rev. Lett. **75**, 193 (1995); **75**, 2786E (1995); Physica A **221**, 80 (1995); C.-K. Hu and C.-Y. Lin, Phys. Rev. Lett. **77**, 8 (1996).

[6] Y. Okabe and M. Kikuchi, Int. J. Mod. Phys. C **7**, 287 (1996).

[7] F.-G. Wang and C.-K. Hu, Phys. Rev. E **56**, 2310 (1997).

[8] C.-Y. Lin, C.-K. Hu, and J.-A. Chen, J. Phys. A **31**, L111 (1998); C.-Y. Lin and C.-K. Hu, Phys. Rev. E **58**, 1521 (1998).

[9] C.-K. Hu, in *Statistical Physics: Experiments, Theories, and Computer Simulations*, edited by M. Tokuyama and I. Oppenheim (World Scientific, Singapore, 1998), p. 83; C.-K. Hu, J.-A. Chen, and C.-Y. Lin, Physica A **266**, 27 (1999).

[10] Y. Okabe, K. Kaneda, M. Kikuchi, and C.-K. Hu, Phys. Rev. E **59**, 1585 (1999).

[11] C.-K. Hu, Phys. Rev. B **46**, 6592 (1992).

[12] R. P. Langlands, C. Pichet, Ph. Pouliot, and Y. Saint-Aubin, J. Stat. Phys. **67**, 553 (1992).

[13] K. Binder, Z. Phys. B **43**, 119 (1981).

[14] C.-K. Hu, Phys. Rev. B **29**, 5103 (1984); **29**, 5109 (1984); for a review, see C.-K. Hu, in *Computer-Aided Statistical Physics*, edited by C.-K. Hu (AIP, New York, 1992), p. 79.

[15] 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).

[16] C.-K. Hu, Physica A **189**, 60 (1992); C.-K. Hu and J.-A. Chen, *ibid*. **199**, 198 (1993).

[17] U. Wolff, Phys. Rev. Lett. **60**, 1461 (1988).

[18] The definition of the metric factor D_1 is different in Ref. [6], where t is defined by $T - T_c$.

[19] G. Kamieniarz and H. W. Blöte, J. Phys. A **26**, 201 (1993).

[20] In Ref. [5], Hu and Lin used R and $C(R)$ to represent a and $\langle n \rangle$, respectively.

[21] M. Aizenman, Nucl. Phys. B **485**, 551 (1997); J.-P. Hovi and A. Aharony, Phys. Rev. E **56**, 172 (1997); J. Cardy, J. Phys. A **31**, L105 (1998).

[22] C.-K. Hu, Phys. Rev. B **44**, 170 (1991).