Histogram Monte Carlo renormalization-group method for percolation problems

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We present a histogram Monte Carlo method to calculate the existence probability E_p, the percolation probability P, and the mean-cluster size S for percolation problems as continuous functions of the bond or site probability p. We then use E_p and P in a percolation renormalization-group method to calculate the critical point and exponents. Our method gives quite accurate results for percolation problems.

In recent decades, much effort has been devoted to the study of percolation,[1–4] including random percolation,[5–11] and correlated percolation.[12–21] The simplest example of percolation is the bond random or site random percolation models on lattices.[3] Although such models are very simple, there are only a few exact results for their critical behavior and no exact results for their global behavior on nontrivial lattices. In order to study the global and critical properties of the random percolation problem, various numerical methods have been used, including Monte Carlo simulation method,[3] transfer matrix method,[7] large-cell renormalization-group transformation,[6] coherent anomaly method,[8] generation of large clusters near critical point,[9,10] finite-size scaling,[11] etc. In this paper we propose a method to study percolation problems. Instead of calculating the percolation probability P, the mean-cluster size S, etc., at various discrete bond or site occupation probabilities p, we use the Monte Carlo simulation method to calculate the histograms of various important quantities from which the percolation probality P, the mean clusters S, and the existence probability E_p (to be defined below) for finite systems at any bond or site occupation probability p may be calculated. We then use E_p and P for different system sizes to formulate a percolation renormalization-group transformation equation to obtain critical point p_c, the thermal scaling power y_t, and the field-scaling power y_h from which various critical exponents of the percolation problems may be obtained. Our method may be applied to both bond and site percolation problems. However, for the sake of simplicity we will present the method in terms of bond random percolation model. The extension to site random percolation model is straightforward. At the end of the paper we will discuss the extension of the method to correlated percolation models corresponding to spin models[14,15] and hard-core particle models.[17] We will also compare our method with other methods for studying phase transitions.[22]

In the bond random percolation model (BRPM) on a lattice G of N sites and E nearest-neighbor bonds, each bond of G is occupied with a probability p, where $0 \le p \le 1$. The probability weight for the appearance of a subgraph G' of $b(G')$ occupied bonds is given by

$$\pi(G',p) = p^{b(G')}(1-p)^{E-b(G')}. \tag{1}$$

The lattice sites connected by occupied bonds are said to be in the same cluster. The cluster which extends from one side of G to the opposite side of G is called a percolating cluster. The subgraph which contains at least one percolating cluster is called a percolating subgraph and will be denoted by G'_p. The subgraph which does not contain any percolating cluster is called a nonpercolating subgraph and will be denoted by G'_f. The existence probability $E_p(G,p)$, the percolation probability $P(G,p)$, and the mean-cluster size $S(G,p)$ of the BRPM on G are given by

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

$$P(G,p) = \sum_{G'_p \subseteq G} \pi(G'_p,p) N^*(G'_p)/N, \tag{3}$$

$$S(G,p) = \sum_{G' \subseteq G} \pi(G',p) \sum_c n_c^2/N, \tag{4}$$

where $\pi(G'_p,p)$ and $\pi(G',p)$ are defined by Eq. (1). The sums in Eqs. (2) and (3) are over all G'_p of G; $N^*(G')$ is the total number of lattice sites in the percolating clusters of G. The first sum in Eq. (4) is over all G' of G; the second sum in Eq. (4) is over all nonpercolating clusters of G' and n_c is the total number of lattice sites in the cluster c of G'. The result of the second sum in Eq. (4) will be denoted by $C_s(G')$. $E_p(G,p)$ will be useful in the percolation renormalization-group calculation of p_c and y_t. Now we proceed to use a histogram Monte Carlo simulation method to calculate E_p, P, and S.

The E nearest-neighbor bonds of G will be labeled by $i = 1, 2, 3, \ldots, E$ in the following. To save computer time of generating random numbers, we generate G' in the following way. To each nearest-neighbor bond of G, say the ith bond, we assign a random number r_i. Such random numbers constitute a random vector of length E: $V = (r_1, r_2, r_3, \ldots, r_E)$. We then consider a se-

quence of bond probabilities of increasing magnitudes: $0 \le p_1 < p_2 < p_3 \cdots < p_w \le 1$. For given p_j, $1 \le j \le w$, if $r_i \le p_j$, then the corresponding ith bond of G is occupied. In this way we generate a bond subgraph G' for each p_j. The total number of occupied bonds in G', $b(G')$, may be calculated easily. The multiple labeling technique of Hoshen and Kopelman[23] is applied to G' to calculate the cluster-size distribution of nonpercolating clusters and the total number of sites in percolating clusters, i.e., $N^*(G')$. Of course, for nonpercolating subgraphs, $N^*(G')$ is 0.

We generate N_R random vectors. For each random vector, we generate w G' corresponding to w different values of p. The data obtained from wN_R G' are then used to construct four arrays of length E with elements $N_p(b)$, $N_f(b)$, $N_{pp}(b)$, and $N_s(b)$, $0 \le b \le E$, which are, respectively, the total numbers of generated percolating subgraphs with b occupied bond, the total number of generated nonpercolating subgraphs with b occupied bonds, the sum of $N^*(G')$ over subgraphs with b occupied bonds, and the sum of $C_s(G')$ over subgraphs with b occupied bonds. In the large number of simulations, we expect that the total number of percolating subgraphs with b occupied bonds, $N_{tp}(b)$, and the total number of nonpercolating subgraphs with b occupied bonds should be proportional to $N_p(b)$ and $N_f(b)$ with the same proportional constant $C(b)$, which may be determined from the following equation:

$$C(b)[N_p(b) + N_f(b)] = N_{tp}(b) + N_{tf}(b) = C_b^E. \quad (5)$$

The existence probability E_p, the percolation probability P, and the mean-cluster size S at any value of the bond occupation probability p may be calculated from the following equations:

$$E_p(G,p) = \sum_{b=0}^{E} p^b(1-p)^{E-b} N_{tp}(b) = \sum_{b=0}^{E} p^b(1-p)^{E-b} C_b^E \frac{N_p(b)}{N_p(b)+N_f(b)}, \quad (6)$$

$$P(G,p) = \sum_{b=0}^{E} p^b(1-p)^{E-b} C_b^E \frac{N_{pp}(b)}{N_p(b)+N_f(b)}, \quad (7)$$

$$S(G,p) = \sum_{b=0}^{E} p^b(1-p)^{E-b} C_b^E \frac{N_s(b)}{N_p(b)+N_f(b)}. \quad (8)$$

Please note that E_p, P, and S of Eqs. (6)–(8) are continuous functions of p. This is quite different from the results obtained by traditional Monte Carlo simulation methods. We have calculated E_p, P, and S for lattices of different linear dimensions L. Typical calculated results are shown in Fig. 1.

Suppose we already carry out histogram Monte Carlo simulations on lattices G_1 and G_2 of linear dimensions L_1 and L_2, respectively, where $L_1 > L_2$. The percolation renormalization-group transformation from lattice G_1 to lattice G_2 is given by the equation

$$E_p(G_2,p') = E_p(G_1,p), \quad (9)$$

which gives the renormalized bond probability p' as a function of p. The fixed point of Eq. (9) gives the critical point p_c, i.e., p_c may be obtained by solving the equation

$$E_p(G_2,p_c) = E_p(G_1,p_c). \quad (10)$$

The thermal scaling power y_t may be obtained from the equation

$$\frac{1}{\nu} = y_t = \frac{(\ln \frac{\partial p'}{\partial p})_{p_c}}{\ln \frac{L_1}{L_2}}. \quad (11)$$

Based on the method of Tsallis, Coniglio, and Schwachheim,[24] Eq. (9) may be iterated to obtain the percolation probability for the thermodynamic system.

It has been shown by Stanley[5] that the field-scaling power y_h for the random percolation is equal to the fractal dimensions D of the percolating cluster at p_c. Therefore y_h and D are given by

$$y_h = D = \frac{\ln \frac{P(G_1',p_c)L_1^d}{P(G_2',p_c)L_2^d}}{\ln \frac{L_1}{L_2}}. \quad (12)$$

Typical calculated values of p_c, y_t, and y_h are shown in Table I, where the exact values for the square lattice[25,26] are also shown for comparison. It obvious from Table I that our method gives quite accurate results. In all calculations we use the periodic boundary condition.

It has been shown that the q-state Potts model (QPM) (Ref. 25) is equivalent to a q-state bond-correlated percolation model (QBCPM) (Ref. 14) in which the probability weight for the appearance of a subgraph G' of $b(G')$ bonds and $n(G')$ clusters is given by

$$\pi(G',p,q) = p^{b(G')}(1-p)^{E-b(G')}q^{n(G')}, \quad (13)$$

where $p = 1 - \exp(-K)$ with K being the normalized nearest-neighbor ferromagnetic coupling constant. The spontaneous magnetization and the magnetic susceptibility of the QPM are related to the percolation probability and the mean-cluster size of the QBCPM, respectively. The histogram Monte Carlo renormalization-group method presented above may be extended to the QBCPM. Instead of calculating four one-dimensional arrays of length E with elements $N_p(b)$, $N_f(b)$, $N_{pp}(b)$, and $N_s(b)$, $0 \le b \le E$, we may calculate four two-dimensional arrays with elements $M_p(b,n)$, $M_f(b,n)$, $M_{pp}(b,n)$, $M_s(b,n)$, $0 \le b \le E$, $0 \le n \le N$, which are, respectively, the total numbers of generated percolating subgraphs with b occupied bond and n clusters, the total number of generated nonpercolating subgraphs with b occupied bonds and n clusters, the sum of $N^*(G')$ over subgraphs with b occupied bonds and n clusters, and the sum of $C_s(G')$ over subgraphs with b occupied bonds and n clusters. Please note that the sum of $M_p(b,n)$ over all n and the sum of $M_f(b,n)$ over all n give $N_p(b)$ and $N_f(b)$, respectively. In the large number

TABLE I. Values of the critical point p_c, the thermal scaling power y_t, and the field-scaling power y_h for the bond random percolation on square lattices calculated by the histogram Monte Carlo renormalization-group method of this paper. The exact values of p_c, y_t, and y_h are 0.5, 0.75, and 1.896, respectively (Ref. 25).

L_1	L_2	N_R	w	p_c	y_t	y_h
16	8	51 200	368	0.5006	0.7651	1.897
20	10	20 000	368	0.4988	0.7492	1.896
28	14	20 000	368	0.5006	0.7623	1.896
32	16	20 000	368	0.5008	0.7403	1.898

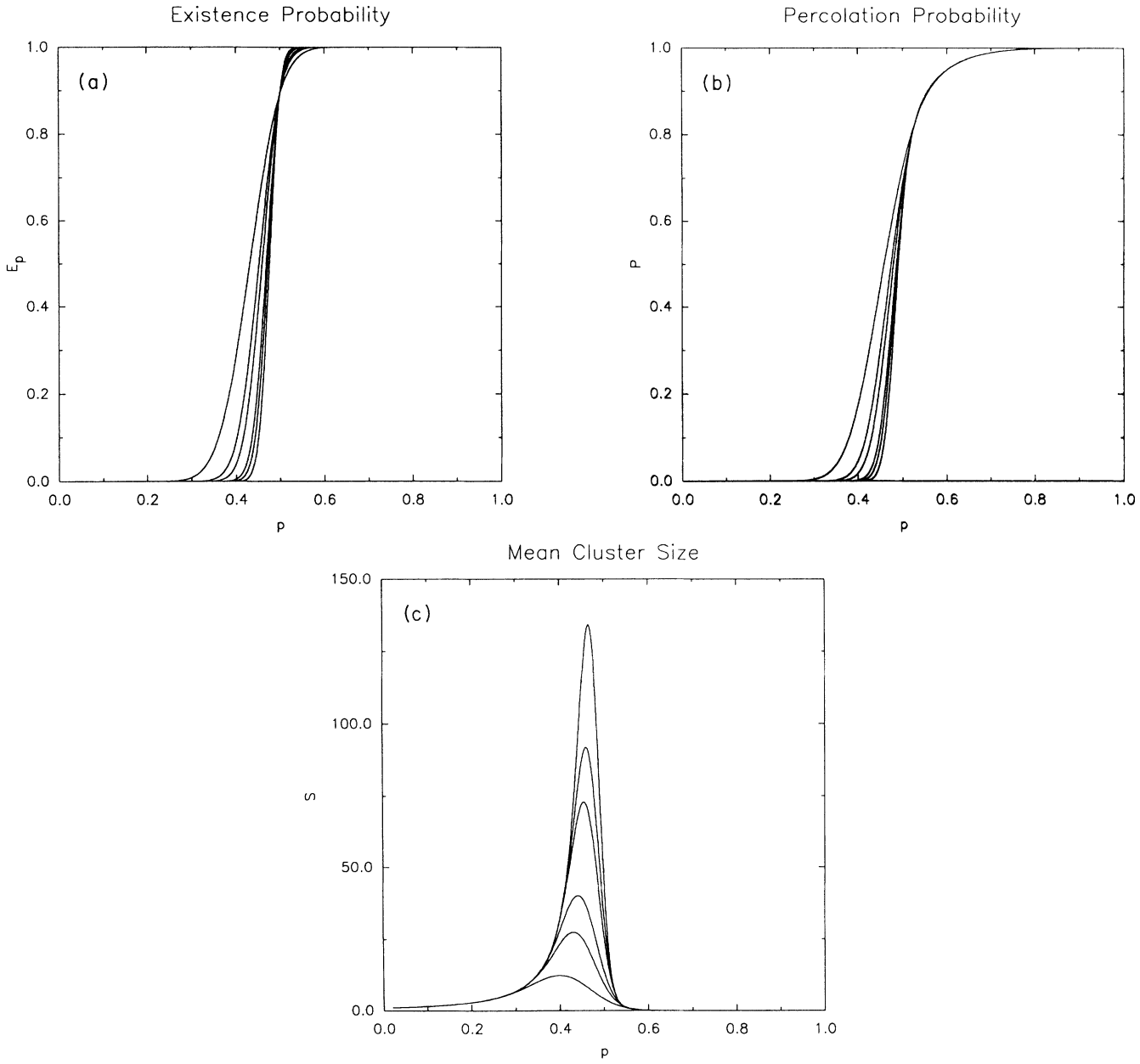

FIG. 1. Results of histogram Monte Carlo simulations for the square lattice of linear dimensions L: 10, 16, 20, 28, 32, and 40. In all cases, we generate 20 000 random vectors and for each random vector we choose 368 different values of bond probability p. (a) Existence probability E_p as a function of p. Near $E_p = 2$, the curves from left to right are for L being 10, 16, 20, 28, 32, and 40, respectively. Note that the intersection of such curves gives the critical point p_c and the slopes at the intersection determine the thermal scaling power y_t. (b) Percolation probability P as a function of p. The curves from left to right are for L being 10, 16, 20, 28, 32, and 40, respectively. (c) Mean-cluster size S as a function of p. Near $p = 0.5$ the curves from down to up positions are for L being 10, 16, 20, 28, 32, and 40, respectively.

of simulations, we expect that the total number of percolating subgraphs with b occupied bonds and n clusters, $M_{tp}(b,n)$, and the total number of nonpercolating subgraphs with b occupied bonds and n clusters should be proportional to $M_p(b,n)$ and $M_f(b,b)$ with the same proportional constant $C(b)$, which may also be determined from Eq. (5). With such normalizations contant, we may easily calculate $E(G,p)$, $P(G,p)$, and $S(G,p)$ and contruct percolation renormalization-group equations to calculate p_c, y_t, y_h, and the thermodynamic free energy for the QPM.[16] Instead of using bond random percolation process to generate subgraphs, one may also use the Swendsen-Wang algorithm[21] to simulate subgraphs for the QPM and QBCPM. With proper normalization of the number of counts by the factor of q to the power of cluster numbers, one may also construct various histograms with the number of occupied bonds b and the number of clusters n as variables and use Eq. (5) to determine absolute magnitudes for various quantities of the QPM and QBCPM. Our preliminary research in this general direction is very encouraging.

It has been shown[17] that phase transitions of lattice hard-core particles are percolation transitions. For such systems one may first consider the site random percolation problem on one sublattice, and then consider the occupation of lattice sites of another sublattice. In this way, it is also possible to contruct a histogram Monte Carlo renormalization-group method for hard-core particles on lattices.

Recently Ferrenberg and Swendsen[22] proposed a histogram Monte Carlo simulation method to calculate the free energy and physical quantities for the QPM. In order to obtain such quantities over a wide range of parameter values, they need to solve a set of coupled nonlinear equations. In our method, we use Eq. (5) to determine the absolute magnitudes and therefore need not solve coupled nonlinear equations.

In summary, we have a histogram Monte Carlo renormalization-group method that may be realized easily, and may give pretty accurate results.

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