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LETTER TO THE EDITOR

Boundary conditions and scaling functions of percolation models

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Abstract. We use a histogram Monte Carlo simulation method to calculate the scaling functions of the existence probability E_p and the percolation probability P of the site percolation model on square lattices with free and periodic boundary conditions. We find that different boundary conditions give quite different scaling functions near the critical region. However, they give the consistent critical point, critical exponents, and the thermodynamic order parameter from renormalization-group calculations. Similar results are found for other percolation models. The implications of our calculated results for some theoretical problems of current interest are discussed.

Finite-size scaling is important in both theoretical [1–5] and experimental [6] studies of critical phenomena. According to the theory of finite-size scaling [1–5, 7], if the dependence of a physical quantity Q of a thermodynamic system on the parameter, t which vanishes at the critical point, may be written as $Q(t) \sim t^a$ near the critical point, then for a finite system of linear dimension L at t, the corresponding quantity $Q(L, t)$ may be written as

$$Q(L, t) \sim L^{-ay_t} F(tL^{y_t}) \tag{1}$$

where y_t (ν^{-1}) is the thermal scaling power and $F(x)$ ($x = tL^{y_t}$) is called a scaling function. When finite-size scaling is valid, the scaled data $Q(L, t)/L^{-ay_t}$ for different values of L fall on the same curve, represented by $F(x)$, if they are plotted as a function of the scaling variable x. Thus, it is important to know the behaviour of the scaling function under various conditions. In this letter, we briefly report our finding for the effect of boundary conditions on the scaling functions of percolation problems which have been of much interest in recent decades [7–15]. Using the histogram Monte Carlo simulation method developed by Hu [16, 17], we calculate the existence probability E_p and the percolation probability P of the site percolation model on the square lattices with free and periodic boundary conditions and with various linear dimensions. For a given boundary condition, the calculated E_p and P have very good scaling behaviour. We find that the scaling functions for the periodic boundary condition and the free boundary condition are quite different near the critical region. However, when we apply the large cell-to-cell Monte Carlo renormalization-group method [16–18] to calculate critical point, critical exponents, and the thermodynamic order parameter, we find that different boundary conditions give consistent results. The implications of our calculated results on some theoretical problems of current interest will be discussed at the end of this letter.

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In the site random percolation model (SRPM) on a d-dimensional lattice G of N sites, each site of G is occupied with a probability p, where $0 \leqslant p \leqslant 1$. The probability weight for the appearance of a subgraph G' of $v(G')$ occupied sites is given by

$$\pi(G', p) = p^{v(G')}(1-p)^{N-v(G')}. \tag{2}$$

The cluster which extends from one side of G to the opposite side of G is called a percolating cluster. The subgraph whose largest cluster is percolating is called a percolating subgraph and will be denoted by G'_p. The subgraph whose largest cluster is not percolating is called a non-percolating subgraph and will be denoted by G'_f. The existence probability $E_p(G, p)$ and the percolation probability $P(G, p)$ for the SRPM on G are given by

$$E_p(G, p) = \sum_{G'_p \subseteq G} \pi(G'_p, p) \tag{3}$$

$$P(G, p) = \sum_{G'_p \subseteq G} \pi(G'_p, p) N^*(G'_p)/N \tag{4}$$

where $\pi(G'_p, p)$ is defined by (2). The sums in (3) and (4) are over all G'_p of G; $N^*(G')$ is the total number of lattice sites in the largest cluster of G. The definitions of G_p, G_f, and $N^*(G')$ in the present paper are different from the corresponding definitions of [16, 17]. The new definitions allow us to save a lot of computing time and therefore we may do the calculations for larger systems.

We choose a sequence of site probabilities of increasing magnitudes: $0 < p_1 < p_2 < p_3 \ldots < p_w < 1$. For a given p_j, $1 \leqslant j \leqslant w$, we generate N_R different subgraphs G'. The data obtained from wN_R different G' are then used to construct three arrays of length N with elements $N_p(v)$, $N_f(v)$, and $N_{pp}(v)$, $0 \leqslant v \leqslant N$, which are, respectively, the total numbers of generated percolating subgraphs with v occupied sites, the total number of generated non-percolating subgraphs with v occupied sites, and the sum of $N^*(G')$ over subgraphs with v occupied sites. In the large number of simulations, we expect that the total number of percolating subgraphs with v occupied sites, $N_{tp}(v)$, and the total number of non-percolating subgraphs with v occupied sites, $N_{tf}(v)$, should be proportional to $N_p(v)$ and $N_f(v)$ with the same proportional constant $C(v)$, which may be determined from the following equation:

$$C(v)[N_p(v) + N_f(v)] = N_{tp}(v) + N_{tf}(v) = C_v^N. \tag{5}$$

where $C_v^N = N!/(N-v)!v!$. The existence probability E_p and the percolation probability P at any value of the site occupation probability p may be calculated from the following equations:

$$E_p(G, p) = \sum_{v=0}^{N} p^v(1-p)^{N-v} N_{tp} = \sum_{v=0}^{N} p^v(1-p)^{N-v} C_v^N \frac{N_p(v)}{N_p(v) + N_f(v)} \tag{6}$$

$$P(G, p) = \sum_{v=0}^{N} p^v(1-p)^{N-v} C_v^N \frac{N_{pp}(v)}{N_p(v) + N_f(v)}. \tag{7}$$

We have used (6) and (7) to calculate the existence probability $E_p(G, p)$ and the percolation probability $P(G, p)$ of the site random percolation model on the square lattices with linear dimensions $L = 32, 64, 128, 256$ and 512. We consider both the free and periodic boundary conditions. Typical calculated results of E_p and P are shown in figures 1(a) and (b), respectively. For the SRPM on the square lattice, it is generally believed that the *exact* y_t and y_h are 0.75 and 1.8958..., [7], and Ziff [14], respectively, have done extensive Monte Carlo simulation on a 1024×1024 lattice to obtain $p_c = 0.592\,746\,0 \pm 0.000\,000\,5$.

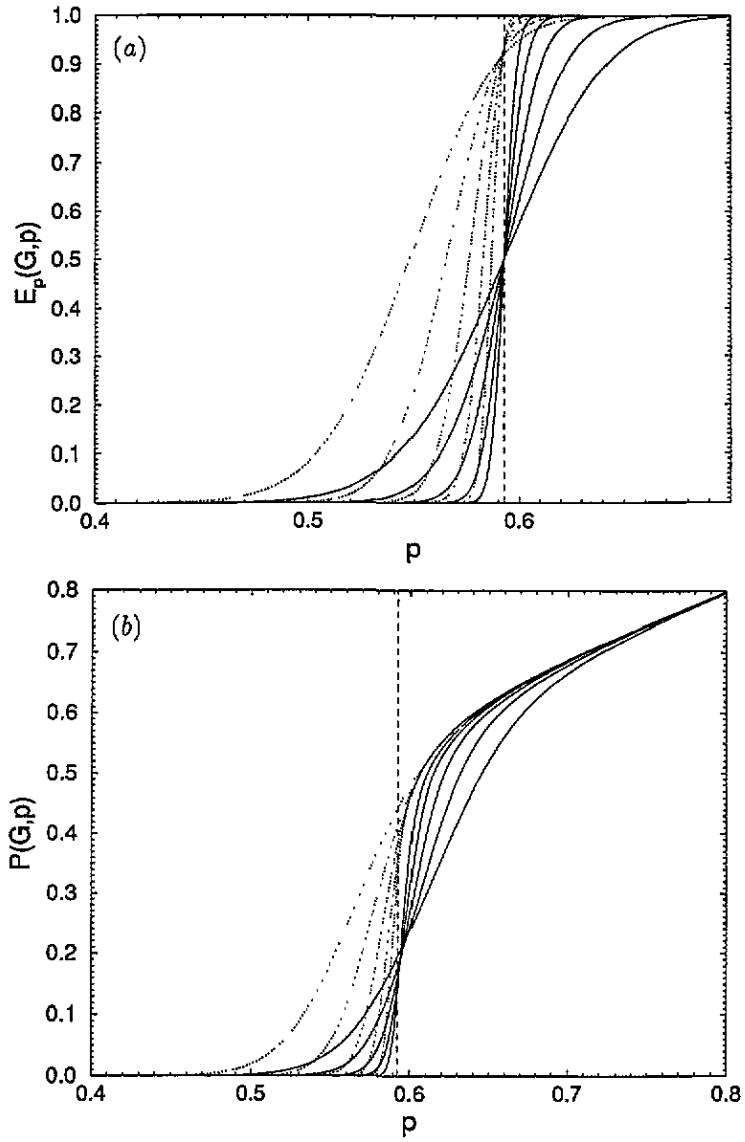

Figure 1. The calculated results for the site random percolation model on square lattices with linear dimensions L: 32, 64, 128, 256, and 512, where the (w, N_R) values are $(420, 9 \times 10^5)$, $(389, 9 \times 10^5)$, $(369, 9 \times 10^5)$, $(369, 1.8 \times 10^5)$, and $(420, 7 \times 10^4)$, respectively, for the free boundary condition. For the periodic boundary condition, 7×10^4 is replaced by 5.6×10^4. (a) E_p as a function of p. For both (a) and (b) the broken vertical line intersects the p-axis at $p_c = 0.5927460$. At p_c, the lower five full curves are for the free boundary condition and the upper five dotted curves are for the periodic boundary condition. (b) P as a function of p. At p_c, the lower five full curves are for the free boundary condition and the upper five dotted curves are for the periodic boundary condition.

Using the exact value of y_t [7] and the numerical value of p_c [14], we have plotted the data for $E_p(G, p)$ represented in figure 1(a) as a function of $x = (p - p_c)L^{y_t}$ in figure 2(a). Since the critical exponent of E_p is zero [7], we need not divide E_p by

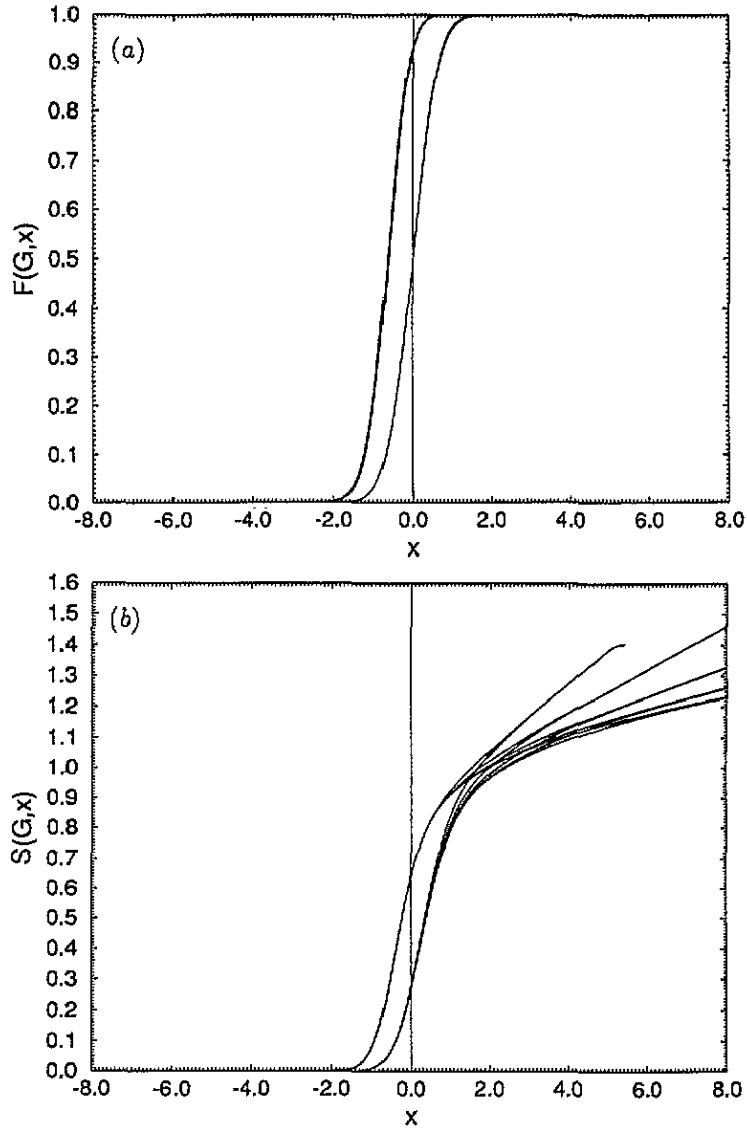

Figure 2. (*a*) The calculated E_p for the square lattice as a function of x, where $x = (p - p_c)L^{y_t}$. The function is the scaling function $F(G, x)$. (*b*) The calculated $P/L^{-\beta y_t}$ for the square lattice as a function of x, where $x = (p - p_c)L^{-y_t}$. The function is the scaling function $S(G, x)$.

the factor L^{-ay_t}, to obtain the scaling function for E_p, which is denoted by $F(G, x)$. It is obvious that $F(G, 0) = E_p(G, p_c)$. Using the same values of y_t and p_c, we have also plotted $P(G, p, q)/L^{-\beta y_t}$ for $P(G, p)$ presented in figure 1(*b*) as a function of $x = (p - p_c)L^{y_t}$ in figure 2(*b*). The scaling function for $P(G, p)$ is denoted by $S(G, x)$.

Figures 2(*a*) and (*b*) show that E_p and P have nice finite-size scaling behaviour. However, the scaling functions for the periodic and the free boundary conditions are quite different. As L approaches very large values, $F(G, 0)$ which equals $E_p(G, p_c)$ approaches 0.5 for the free boundary condition and approaches 0.93 for the periodic boundary condition. The value 0.5 is consistent with the result of conformal field theory [14, 23].

In the previous calculations, a cluster is percolating if it percolates in a given direction, i.e. from top to bottom. We have also studied the case where a cluster is percolating only if it percolates in two directions, i.e. from top to bottom and from left to right [19]. We have found that such a definition gives different scaling functions. For the periodic boundary condition and the free boundary conditions, $F(G, 0)$, i.e. $E_p(G, p_c)$, equals 0.89 and 0.33, respectively, which are smaller than the corresponding values for *one direction* percolation.

The percolation renormalization-group (PRG) transformation from lattice G_1 of linear dimension L_1 to lattice G_2 of linear dimension L_2, where $L_1 > L_2$, is given by the equation [16, 17]

$$E_p(G_2, p') = E_p(G_1, p) \tag{8}$$

which gives the renormalized site probability p' as a function of p. The fixed point of (8) gives the critical point p_c. The thermal scaling power y_t and the field scaling power y_h, which is equal to the fractal dimension D of the percolating cluster at p_c [8, 20], may be obtained from the equations

$$\frac{1}{\nu} = y_t = \frac{\ln(\partial p'/\partial p)_{p_c}}{\ln(L_1/L_2)} \qquad y_h = D = \frac{\ln(P(G_1', p_c)L_1^d/P(G_2', p_c)L_2^d)}{\ln(L_1/L_2)}. \tag{9}$$

We have used the above equations to calculate the critical point p_c, the thermal scaling power y_t, and the field scaling power y_h for the SRPM on the square lattice. For the free boundary condition, we use $w = 420$ and $N_R = 70\,000$ for $L_1 = 512$, and $w = 369$ and $N_R = 180\,000$ for $L_2 = 256$ to obtain $p_c(\text{sq}) = 0.592(8)$, $y_t = 0.7(5)$, and $y_h = 1.89(3)$. For the periodic boundary condition, we use $w = 420$ and $N_R = 56\,000$ for $L_1 = 512$, and $w = 369$ and $N_R = 180\,000$ for $L_2 = 256$ to obtain $p_c(\text{sq}) = 0.592(8)$, $y_t = 0.7(5)$, and $y_h = 1.89(6)$. The two results are consistent. Our numerical results are very close to the exact results [7] or the numerical results of Ziff [14].

With each site of the lattice we may associate an adimensional 'magnetic moment' m_0 and consider the renormalization of m_0 under the PRG transformation to give the renormalized 'magnetic moment' m_0' [21, 22]

$$m_0' P(G_2, p', q) L_2^d = m_0 P(G_1, p, q) L_1^d \tag{10}$$

which means that the total 'magnetization' is preserved after the PRG transformation. After a series of PRG transformations, we have a series of renormalized site probability p, $p^{(1)}(= p')$, $p^{(2)}, \ldots, p^{(n)}$ and the renormalized magnetic moments m_0, $m_0^{(1)}(= m_0')$, $m_0^{(2)}, \ldots, m_0^{(n)}$. The thermodynamic percolation probability of the original systems, $P_\infty(p)$, may be related to the thermodynamic percolation probability of the nth transformed system, $P_\infty(p^{(n)})$, by the equation

$$P_\infty(p) = \frac{m_0^{(n)}}{\lambda^{nd} m_0} P_\infty(p^{(n)}) \tag{11}$$

for $p > p_c$ with $\lambda = L_1/L_2$. In the traditional small-cell RG transformation (RGT) [21, 22], one iterates the RGTs until $p^{(n)}$ approaches the 'lower-temperature' fixed point $p_c = 1$ then $P_\infty(p^{(n)})$ of (11) is given by 1. However, in the large cell-to-cell RGTs considered here, one need only iterate the RGTs until the correlation length of the nth transformed system is smaller than the linear dimensions of the transformed cell. In such a case, the transformed cell may well represent the thermodynamic systems and we may use $P(G_2, p^{(n)})$ to represent $P_\infty(p^{(n)})$ of (11) and obtain [18]

$$P_\infty(p) = \frac{m_0^{(n)}}{\lambda^{nd} m_0} P\left(G, p^{(n)}\right). \tag{12}$$

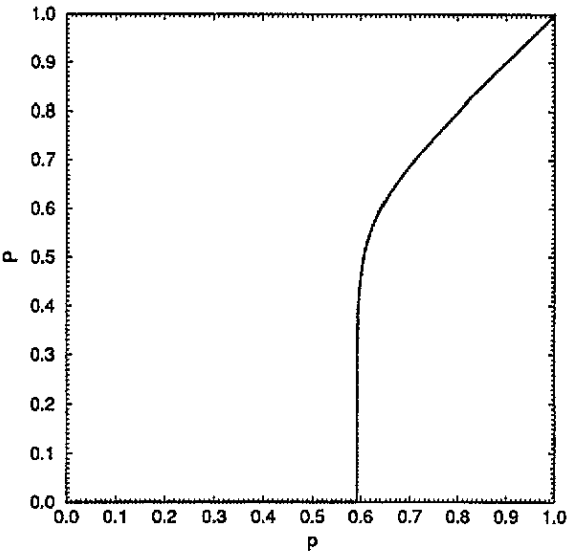

Figure 3. The calculated thermodynamic order parameters $P_\infty(G, p)$ of the site random percolation model on the square lattice. The full and dotted curves are for the free and periodic boundary conditions, respectively.

We have used (12) to calculate the thermodynamic order parameter P_∞ for the SRPM with the free and periodic boundary conditions, which are shown by full and dotted curves in figure 3, respectively. The two calculated results are consistent.

From our calculated results, we may discuss some theoretical problems of current interest. Ziff [14] called the existence probability E_p in our papers [16, 17, 20] the spanning probability and denoted it by $R_L(p)$. In a recent letter [14], Ziff used extensive Monte Carlo simulations to study $R_L(p)$ for a site random percolation model on a square lattice with the free boundary condition. He found that $R_L(p) \to \frac{1}{2}$ as $L \to \infty$ in agreement with Cardy's recent result [23] but not with renormalization-group (RG) theory. He pointed out that the RG transformation (RGT) $p' = R_L(p)$ cannot give the expected result $R_L(p_c) = 0.5$ as $L \to \infty$. We think this is due to the fact that the *cell-to-site* RGT used by Ziff is not a good RGT in the sense that the transformed system, i.e. a site, cannot represent the original system well. In [16], we considered the RGT from a lattice G_1 of linear dimension L_1 to a lattice G_2 of the linear dimension L_2, where $L_1 > L_2$, and wrote the RGT equation as (8) of the present paper. For sufficiently large values of L_1 and L_2 so that $E_p(G_1, p)$ and $E_p(G_2, p)$ have good scaling behaviour near the critical point, we expect that at the critical point p_c determined by (8) which is represented as the intersection of two curves in figure 1(*a*), $E_p(G, p_c)$ for the free boundary condition will approach $\frac{1}{2}$ when $L \to \infty$ as Ziff did [14]. The curves of the free boundary conditions in figure 1(*a*) support this idea. This also shows that one may get $E_p(G, p_c) = 0.5$ from the large cell-to-cell RGT of (8) and one need not use the large parameter space RG transformation considered by Aharony and Hovi [24].

Hu and Chen have used the histogram Monte Carlo simulation method [16, 17] to calculate the scaling functions of the bond percolation on the square, the honeycomb, the Kagome, the plane triangular, the simple cubic, and the body-centred cubic lattices with the periodic boundary condition [20, 25, 26]. The results show that lattices with the same space dimensions may not have the same value of E_p at p_c, e.g. the scaling functions of

figures 4(a) and 6(a) of [25] have different values at $x = 0$, corresponding to the critical point p_c. The calculations of scaling functions for the site percolation on various two- and three-dimensional lattices with free and periodic boundary conditions also show similar results [27]. Using the histogram Monte Carlo simulation method [16, 17], Hu and Chen [28] have found that the scaling functions of percolation problems depends on the ratio of the horizontal linear dimension a and vertical linear dimension b of the lattices. Using the idea of Langlanda *et al* [29], we may adjust the ratio a/b for various lattices on the same space dimensions so that different lattices give the same value of $E_p(G, p_c)$, i.e. $F(G, 0)$. We use the histogram Monte Carlo simulation method [16, 17] to calculate such a/b ratios and the scaling functions for various two- to five-dimensional lattices.

Cardy [23] has used the conformal field theory to calculate exactly the crossing probability for bond percolation on rectangles. His results agree very well with the numerical results of Langlanda *et al* [29]. It is valuable to extend such a study to the site percolation problem using the histogram Monte Carlo simulation method [16–18].

In summary, the value of E_p at p_c, i.e. $F(G, 0)$, depends on the boundary condition and the shape of the lattice, and also on the rule used to identify the percolating cluster. The histogram Monte Carlo simulation method [16, 17] is useful for identifying the *universality classes* of $E_p(G, p_c)$, which is of much current interest [30, 31], and for obtaining the scaling functions for E_p and P, and for calculating the critical point, critical exponents, and the thermodynamic order parameter.

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