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Site–Bond Percolation Problems

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We study a percolation process in which both sites and bonds are randomly blocked, independent of each other. In the Bethe lattice, the exact solution for the percolation threshold is found to be a hyperbola in the x–p plane, where x and p are the respective probabilities of each site and bond being unblocked. Percolation threshold for a square and a simple cubic lattice is obtained by computer simulation. We also present a result obtained by a real-space renormalization group technique for the square lattice.

KEY WORDS: Site–bond percolation; percolation threshold.

1. INTRODUCTION

The percolation model has achieved certain success in explaining some physical properties of random systems.[1] Usually, the percolation model in a lattice is classified into two categories, namely, site model and bond model. In the former model sites are randomly blocked, and in the latter bonds are randomly blocked. Some real physical systems, however, have blockage in both sites and bonds, where unbroken bonds act as communication links between unblocked sites. For example, Ising model with randomly missing spins and vanishing exchange interactions, and the problem of spreading of epidemic diseases are considered to be among this kind of problem. In fact, there have been several works on site–bond percolation problem where sites and bonds are randomly blocked, independent of each other, with probabilities $(1 - x)$ and $(1 - p)$, respectively. The dependence of critical temperature on site–bond occupation probabilities for a Heisenberg ferromagnet on a fcc lattice was studied by Brown *et al.*[2]

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using the ratio and Padé approximant methods. Low-density series expansion method was used by Agrawal *et al.*[3] to study uncorrelated site–bond percolation on a square lattice. Hoshen *et al.*[4] studied the site–bond percolation problem in a square lattice by computer simulation. Their results for the percolation threshold showed large fluctuations possibly due to their criterion for percolation. Similar Monte Carlo methods have been used by Heermann and Stauffer[5] and Ottavi[6] in studying Ising-like correlated site–bond percolation in a simple cubic lattice and a square lattice. Using a generalized star–triangle transformation, Kondor[7] obtained explicit formulas for the site–bond percolation threshold for triangular and honeycomb lattices. Coniglio and Klein[8] and Wu[9] established the connection between the dilute Potts model and the site–bond percolation problem. Furthermore, McGurn[10] presented a technique to map site–bond disorder problems on Ising systems onto a certain class of decorated lattice problems. He used the zero-temperature magnetization to obtain an approximation to the percolation probability and deduced the site–bond percolation threshold for the honeycomb lattice. A correlated site–bond percolation model has also been used in the study of polymer gelation.[11,12]

In this paper, we study the uncorrelated site–bond percolation problem in the Bethe lattice, the square, and the simple cubic lattices. In Section 2 we derive the exact solution to the site–bond percolation problem in the Bethe lattice. We shall follow closely the generating function technique[13] and show that the percolation threshold in the x–p plane is given by a hyperbola $xp = 1/\sigma$, where $z = \sigma + 1$ is the coordination number of the Bethe lattice. We call this threshold the critical percolation hyperbola. This hyperbola is in fact the infinite temperature limit of the gelation threshold Eq. (6) of Ref. 11 obtained there by a different method. We study in Section 3 the site–bond percolation model in the square and simple cubic lattices using a Monte Carlo technique. In the simple cubic lattice, the percolation transition line in the x–p plane exhibits hyperbolic behavior. In Section 4, we discuss similarities and differences with earlier results and mention a result obtained by a real-space renormalization group technique for the square lattice.

2. THE BETHE LATTICE

We define a cluster as a set of unblocked sites linked to one another through unbroken bonds. A cluster can be characterized by its size and number of perimeters isolating the cluster. The cluster size is measured by the number of sites it contains. (We can also use the number of bonds in the cluster to measure the cluster size, but results should be independent of

definition.) The perimeters of a cluster in the site–bond percolation problem can be either broken bonds or blocked sites. A cluster can be isolated in two ways: (a) bond is unbroken but site is not, probability of which is py; (b) bond is broken, probability of which is q.

Here, $y = 1 - x$ is the probability of a blocked site and $q = 1 - p$ is the probability of a broken bond. Thus, the probability of having a cluster of size s with t perimeters is given by

$$x^s p^{s-1}(py + q)^t \tag{2.1}$$

Note the exponent $s - 1$ of p since the number of bonds inside the cluster is always one less than the cluster size for the Bethe lattice.

Denote by $a_{s,t}$ the number of distinct clusters of size s and perimeter t which contain a given site. Then the probability of an unblocked site belonging to such clusters is given by

$$a_{s,t} x^s p^{s-1}(py + q)^t \tag{2.2}$$

The topological degeneracy factor $a_{s,t}$ does not depend on the model one is using.

The total probability that a site belongs to a finite size cluster is then

$$F(x, p) = \sum_{s,t} a_{s,t} \frac{1}{p} (xp)^s (1 - xp)^t \tag{2.3}$$

The percolation probability that a site belongs to an infinite cluster will be

$$R(x, p) = x - F(x, p) \tag{2.4}$$

We note that below a certain percolation threshold, all clusters are of finite size and the total probability of a site belonging to a finite cluster is simply the probability that the site is unblocked. Consequently, we must have

$$F(x, p) = x \tag{2.5}$$

Therefore, the percolation threshold is defined as $\inf\{x \mid R(x, p) > 0\}$ for any p in $[0, 1]$, or equivalently $\inf\{p \mid R(x, p) > 0\}$ for any x in $[0, 1]$.

Now we define the generating function

$$A(u, v) := \sum_{s,t} a_{s,t} u^s v^t \tag{2.6}$$

so that

$$F(x, p) = \frac{1}{p} A(xp, 1 - xp) \tag{2.7}$$

We further define a configurational generating function

$$K(u, v) := \sum_{s,t} \frac{1}{s} a_{s,t} u^s v^t \tag{2.8}$$

which gives the relation

$$A(u,v) = u\frac{\partial K(u,v)}{\partial u} \tag{2.9}$$

For the Bethe lattice, a unique relation between s and t exists,

$$t = s(\sigma - 1) + 2 \tag{2.10}$$

where $\sigma = z - 1$ is the connectivity of the lattice. Using this relation, we can rewrite the configurational generating function (2.8) as

$$K(u,v) = v^2 B_\sigma(\eta) \tag{2.11}$$

where $\eta = uv^{\sigma-1}$, and $B_\sigma(\eta)$ is the fundamental Bethe lattice generating function given by

$$B_\sigma(\eta) = \sum_{s,t} \frac{1}{s} a_{s,t}\eta^s \tag{2.12}$$

The explicit form of the fundamental Bethe generating function is known to be[13,14]

$$B_\sigma(\eta) = \frac{2P^* - (\sigma+1)P^{*2}}{2(1-P^*)^2} \tag{2.13}$$

where $P^*(\eta)$ is a solution to

$$P^*(1-P^*)^{\sigma-1} = \eta \tag{2.14}$$

satisfying

$$\lim_{\eta\to 0} P^*(\eta) = 0 \tag{2.15}$$

Equations (2.5), (2.9), and (2.11) lead to

$$F(x,p) = x(1-xp)^{\sigma+1}\frac{dB_\sigma(\eta)}{d\eta} \tag{2.16}$$

where the derivative is evaluated at

$$\eta = xp(1-xp)^{\sigma-1} \tag{2.17}$$

After a simple algebraic manipulation, the density of finite clusters Eq. (2.16) is reducible to

$$F(x,p) = \frac{P^*}{p}\left(\frac{1-xp}{1-P^*}\right)^2 \tag{2.18}$$

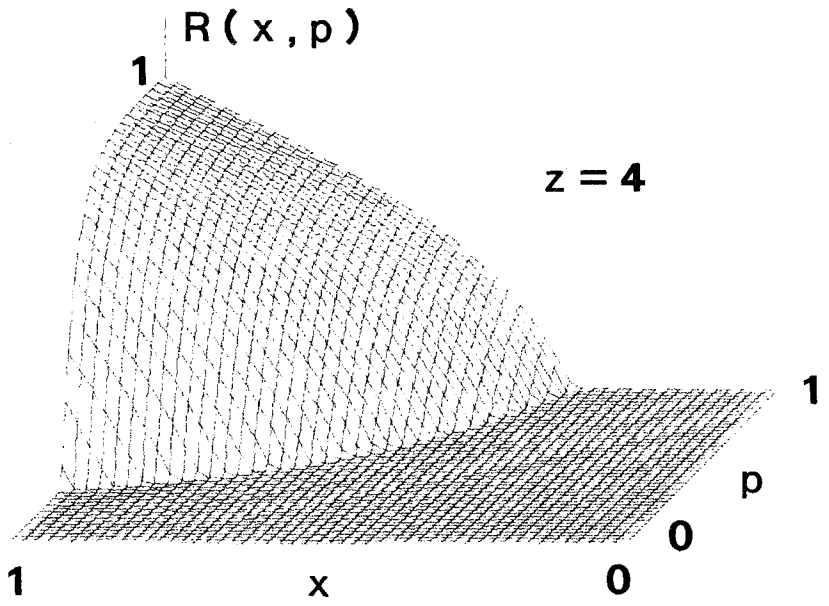

Fig. 1. Perspective view of the site–bond percolation probability for the Bethe lattice with coordination number $z = 4$. x and p are the probability of a site and a bond being unblocked, respectively.

and hence that of infinite cluster is reduced to

$$R(x, p) = x\left[1 - \frac{P^*}{xp}\left(\frac{1 - xp}{1 - P^*}\right)^2\right] \tag{2.19}$$

Noting that η defined in Eq. (2.17) as a function of xp attains its maximum value at $xp = 1/\sigma$, we have, from Eqs. (2.14), (2.15), and (2.17),

$$P^* = xp \tag{2.20}$$

when $xp < 1/\sigma$. When $xp > 1/\sigma$, we find $P^* = 1 - xp$ for $\sigma = 2$, and $P^* = \{2 - xp - [xp(4 - 3xp)]^{1/2}\}/2$ for $\sigma = 3$ and so forth. Figure 1 shows the perspective view of the percolation probability surface $R(x, p)$ calculated through Eq. (2.19) for $z = 4$. The percolation threshold defined below Eq. (2.5) is found to be a hyperbola $(xp)_c = 1/\sigma$. If we set $x = 1$ ($p = 1$), this hyperbola correctly reduces to the usual critical percolation probabilities for the pure bond (site) problem, namely, $p_c = 1/\sigma$ ($x_c = 1/\sigma$). The critical percolation hyperbola for various σ is plotted in Fig. 2.

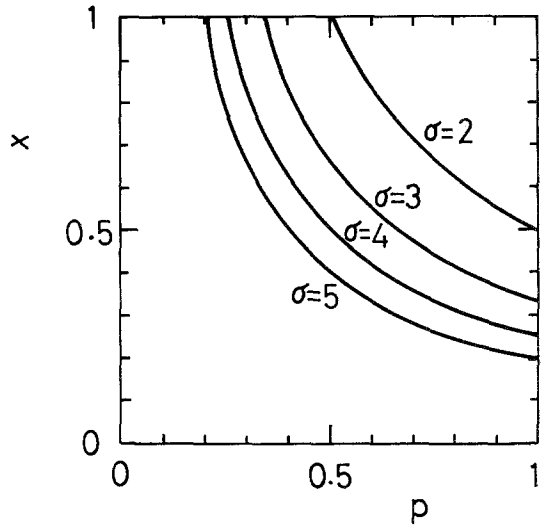

Fig. 2. Percolation threshold of the site–bond percolation problem in the Bethe lattice with various connectivities. Note the connectivity σ is one less than the coordination number z.

The mean cluster size is defined as

$$S(x, p) = \frac{\sum_{s,t} s a_{s,t} (1/p)(xp)^s (1 - xp)^t}{F(x, p)} \tag{2.21}$$

Using the generating function $B_\sigma(\eta)$, we can rewrite it as

$$S(x, p) = 1 + P^*(1 - P^*)^{\sigma - 1} \left\{ \frac{d}{dP^*} \ln \left[\frac{dB_\sigma(\eta)}{d\eta} \right] \right\} \cdot \frac{dP^*}{d\eta} \Bigg|_{\eta = xp(1-xp)^{\sigma-1}}$$

Further simplification gives

$$S(x, p) = \frac{1 + P^*}{1 - \sigma P^*} \tag{2.22}$$

The mean cluster size $S(x, p)$ diverges on the critical percolation hyperbola. Critical indices of the percolation probability and the mean cluster size are the same as that of the pure site or bond problem and do not depend on how one approaches the critical hyperbola.

3. SQUARE AND SIMPLE CUBIC LATTICES

In this section we present results of computer simulation on the site–bond percolation threshold for square (100×100) and simple cubic

($20 \times 20 \times 20$) lattices with fixed boundary conditions. We first used a pseudorandom number generator to generate randomly distributed blocked sites and broken bonds. Then, we connected two adjacent unblocked sites if they shared a common unbroken bond. The system was assumed to have an "infinite" cluster if there exists at least one connected channel of unblocked sites which extends from one edge to the opposite edge of the square lattice (for the simple cubic lattice, from one face to the opposite face). We changed the probability x (or p) for a given p (or x) by a step size 0.001. The critical percolation probability x_c for a given p (or p_c for a given x) was determined as the smallest x (or p) where the system has an infinite cluster. For the square lattice, we ran five samples, and for the simple cubic lattice, 10 samples. The percolation threshold was determined as an average of critical probabilities over these samples.

The solid circles in Fig. 3 show the percolation threshold for the square and simple cubic lattices determined by the foregoing procedure. The standard deviation for the square lattice is at most 0.01, within the size of the solid circles. For the simple cubic lattice, the standard deviations are shown by bars through the solid circles. When $p = 1$ or $x = 1$, the present results shown in Table I agree with the values for the pure site or bond problem known in the literature[15] to within 1%. In Fig. 3, we also show data obtained by other authors for comparison.

The critical percolation line appears to be fitted by a hyperbola

$$(x - 0.123)(p + 0.069) = 0.499 \tag{3.1}$$

for the square lattice and

$$(x - 0.054)(p + 0.036) = 0.270 \tag{3.2}$$

for the simple cubic lattice. They are shown by the solid curves in Fig. 3. The fitting of the hyperbola was done using the two end points (i.e., the pure site or bond case) and the point on the diagonal $x = p$. However, the fitting for the square lattice is not as good as that for the simple cubic lattice.

Table I. Percolation threshold for the pure site and bond problems.

	Square		Simple cubic	
	Bond	Site	Bond	Site
Ref. 15	0.500[a]	0.593	0.249	0.311
Present result	0.500 ± 0.005	0.586 ± 0.008	0.249 ± 0.010	0.315 ± 0.011

[a] Exact result.

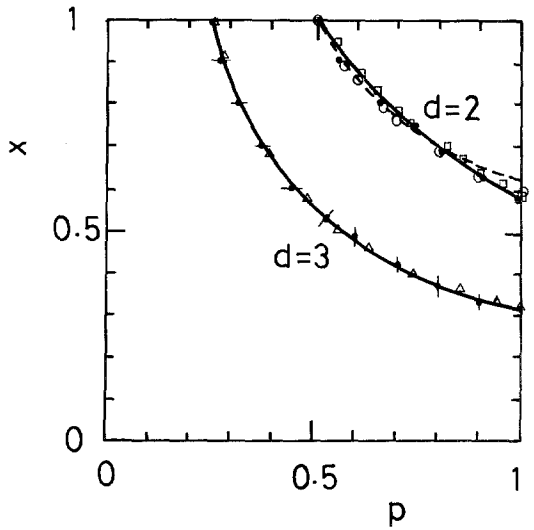

Fig. 3. Percolation threshold of the site–bond percolation problem in the square and simple cubic lattices. Solid circles are the results obtained by present computer simulation and bars denote the standard deviation. For the square lattice, the standard deviation is within the size of the solid circle. Solid lines are hyperbolas which interpolate data at three points as explained in the text. The broken line is the fixed point solution to Eq. (4.1) obtained from a real space renormalization group for the square lattice. For comparison, results found by Agrawal *et al.*[3] (□) and Ottavi[6] (○) for the square lattice, and Heermann and Stauffer[5] (△) for the simple cubic lattice are shown. Open circles are extracted from the continuous curve shown in Fig. 2 of Ref. 6 and open squares and triangles are typical data shown in Fig. 1 of Ref. 3 and Fig. 1 of Ref. 5, respectively.

4. DISCUSSION

We have studied in this paper the site–bond percolation problem in the Bethe lattice, the square, and the simple cubic lattices. We obtained the exact result of the percolation probability, the percolation threshold and the mean cluster size for the Bethe lattice. The percolation threshold is shown to be a hyperbola $(xp)_c = 1/\sigma$. Therefore, sites and bonds in the Bethe lattice play a symmetric role in the percolation process. Our result agrees with Eq. (6) of Ref. 11 in the case of a single monomer chain at the infinite temperature limit. Critical indices for the percolation probability and the mean cluster size at the threshold are the same as the pure site or bond problem in the Bethe lattice, indicating the site–bond universality.

For the square and simple cubic lattices, we obtained the site–bond percolation threshold by making use of computer simulation. The present

result for the square and simple cubic lattices are in good agreement with results obtained in Ref. 3, 5, and 6. Our data for the square lattice as well as for the simple cubic lattice can be fitted by a hyperbola. Such hyperbolic behavior was conjectured by Heermann and Stauffer.[5] The hyperbolic behavior of the site–bond percolation threshold does not manifest itself in the case of the honeycomb and triangular lattices as was shown by Kondor.[7] We shall see later that the real-space renormalization group technique does not give hyperbolic percolation threshold for the square lattice. According to the scaling theory,[15] both the pure site and bond percolation threshold in the d-dimensional hypercubic lattice are given by $1/(2d-1) = 1/(z-1)$ as the dimensionality d becomes large. This coincides with the critical probability for the pure site or bond percolation in the Bethe lattice. We expect, thus, the hyperbolic nature of the site–bond percolation threshold will hold asymptotically for the hypercubic lattice in higher dimensions.

Finally, we mention a result for the square lattice predicted by a real space renormalization group. We generalized the renormalization transformation used by Reynolds *et al.* [Fig. 3(a) in Ref. 16] for the pure bond percolation to the site–bond problem. The real-space renormalization group transformation leads to

$$p'x' = p^2x^2\left[2 + 2px(1-p) - p^2x^2(3-2p)\right] \tag{4.1}$$

where p' and x' are the rescaled probabilities. The fixed point solution to Eq. (4.1) is given by

$$xp = 2/\left[1 + (13-8p)^{1/2}\right] \tag{4.2}$$

which is shown by the broken line in Fig. 3. It gives $p_c = 0.500$ when $x = 1$ and $x_c = (\sqrt{5}-1)/2 \sim 0.618$ when $p = 1$. The solution (4.2) is in good agreement with the result of our computer simulation when $p \lesssim 0.8$ and somewhat deviates when $p \gtrsim 0.8$.

It should be mentioned that Eq. (4.1) is identical to Eq. (2) of Ref. 17. The recursion equation (4.1) has been derived by requiring that a classical fluid can go through the cell either horizontally or vertically. We consider this condition sufficient to determine the critical line. In fact, Eq. (4.1) reduced to Eq. (12) of Ref. 16 for pure bond case and to Eq. (4.4) of Ref. 18 for pure site case.

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