High-Density Percolation: Exact Solution on a Bethe Lattice

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A new percolation problem is posed where the sites on a lattice are randomly occupied but where only those occupied sites with at least a given number m of occupied neighbors are included in the clusters. This problem, which has applications in magnetic and other systems, is solved exactly on a Bethe lattice. The classical percolation critical exponents $\beta = \gamma = 1$ are found. The percolation thresholds vary between the ordinary percolation threshold $p_c(m = 1) = 1/(z - 1)$ and $p_c(m = z) = [1/(z - 1)]^{1/(z-1)}$. The cluster size distribution asymptotically decays exponentially with n, for large n, $p \neq p_c$.

1. INTRODUCTION

In the usual percolation model[1-3] one considers the sites of a lattice to be randomly occupied (or vacant) with a probability p (or $1 - p$). This model is useful for the physical properties of many real systems. For example, some quenched, dilute ferromagnets and antiferromagnets behave at low temperatures like a system of independent magnetic clusters of atoms which display a critical behavior near percolation threshold that is characterized by the singular behavior of the moments of the cluster size distribution.[4]

On the other hand, there are several, mostly unexplored, systems where physical properties are affected by a percolation-like growth of the high-density regions. Specifically, a model of high-density percolation on a lattice is obtained by randomly occupying (or not) each site with probability p (or $1 - p$) but then restricting one's attention to only those regions of the lattice where there is a high density of occupied sites. At a higher critical concentra-

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tion (than that of ordinary percolation) these high-density regions merge to form a high-density, infinite cluster. Let us consider briefly two physical examples where such concepts may be important.

First, there are systems of magnetic impurities in metallic lattices where the formation of a localized magnetic moment depends upon the local environment about the impurity site in an essentially discontinuous way. The model for these systems was first proposed by Jaccarino and Walker,[5] who studied Fe impurities in $Nb_{1-c}Mo_c$ body-centered cubic alloys and found that the Fe impurity develops a local magnetic moment only if at least seven of its neighbors are Mo atoms. They also found that Co impurities in $Rh_{1-c}Pd_c$ face-centered cubic alloys require at least two Pd neighbors for the formation of a moment. In these systems, the magnetic moment is essentially either zero or some maximum value, depending upon the local environment.

More recently, similar results have been reported in binary alloys,[6] such as Ni_pCu_{1-p}, Co_pRe_{1-p}, and Ni_pV_{1-p}. In these cases, a magnetic site develops a local moment whenever it is surrounded by sufficiently many other magnetic near neighbors. In these binary systems as the concentration p of magnetic sites increases, the regions with magnetic moments grow and merge until, at a critical concentration $p_c(m)$ (where m is the critical number of magnetic
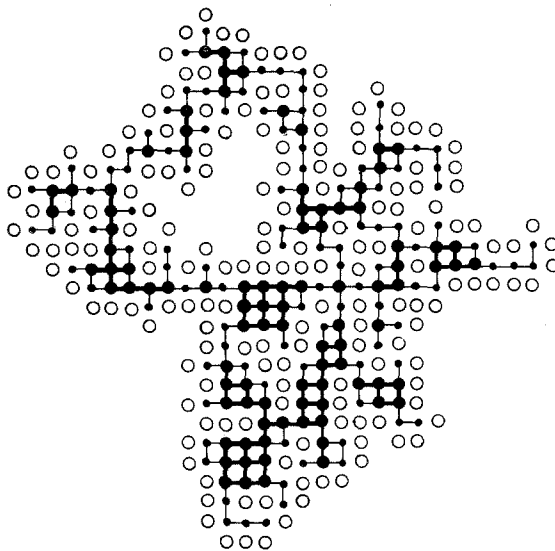

Fig. 1. Example of a single cluster of occupied sites (solid circles, both sizes) and its vacant perimeter (open circles) on a square lattice. This cluster contains several smaller 3-clusters of sites (large solid circles) in its high-density regions.

near neighbors) an infinite magnetic cluster appears and the system becomes ferromagnetic. This critical concentration varies from about 0.45 to about 0.87 in the systems studied thus far and depends on the lattice structure and the critical number of neighbors m. Examples of two-dimensional magnetic clusters are illustrated in Fig. 1, $m = 3$ on the square lattice.

Second, there is the somewhat less clear possible example of the liquid-glass transition. Turnbull and Cohen[7] have previously developed a free-volume model for molecular transport in dense fluids. The extension to describe the thermodynamic properties has been developed by Cohen and Grest[8] using ideas from percolation theory. In this model, the atom moves in a volume v, which is either solid-like or liquid-like, depending on its value. Those liquid-like cells which are surrounded by a minimum number of other liquid-like cells form clusters and can exchange volume freely. The communal entropy of the system depends upon the distribution of liquid clusters. The density p is a function of temperature and as p approaches p_c there is a sharp freezing out of the entropy as the infinite cluster disappears, resulting in a drop in the heat capacity. The critical concentration p_c is then related to the liquid-glass transition temperature T_g.

In this paper, we shall give a few exact results for high-density percolation on the Bethe lattice to illustrate certain general features of the problem and to clarify the similarities and differences with regard to ordinary percolation.

2. EXACT SOLUTION FOR THE BETHE LATTICE

We shall consider each site of the lattice to be randomly occupied (or vacant) with probability p (or $1 - p$). We then restrict our attention to only those occupied sites each of which has m of its z nearest neighbor sites occupied. Clusters of such sites will be called m-*clusters*, and we shall primarily be concerned with the probability $P_m(n, p)$ that a given occupied site is in an m-cluster of size n. For example, in Fig. 2 the circled occupied site on the
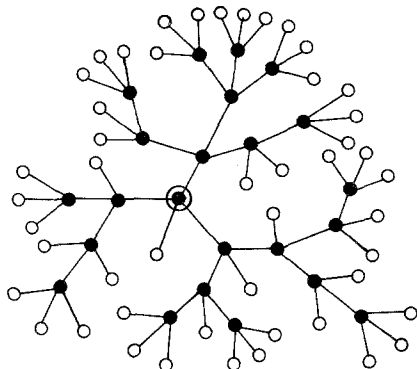

Fig. 2. A cluster of occupied sites (solid circles) and their vacant perimeter sites (open circles). The circled occupied site is part of 1-cluster of 23 sites, a 2-cluster of 12 sites, a 3-cluster of 7 sites, and a 4-cluster of zero sites.
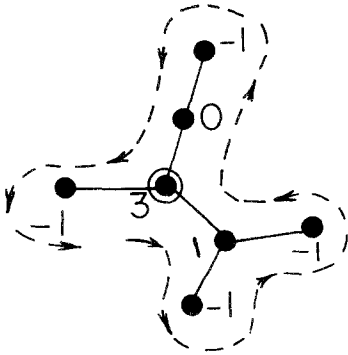
Fig. 3. The 3-cluster of Fig. 2 is reproduced; the valence three of the origin site is labeled along with the valence less two of each other site; the indicated counterclockwise path passes the sites in the order that gives the sequence 3, 1, -1, -1, 0, -1, -1 that labels the cluster class.

$z = 4$ Bethe lattice is in a 1-cluster of size 23, a 2-cluster of size 12, a 3-cluster of size 7, and 4-cluster of size zero.

On a Bethe lattice we can solve this problem exactly by translating it into an equivalent random-walk problem and making use of the substantial literature[9,10] on that subject.

First, we divide the clusters of atoms into classes according to their geometry, as illustrated in the example in Fig. 3, where the 3-cluster of Fig. 2 has been redrawn. In this scheme we begin by labeling the origin (the circled atom) by its valence (number of nearest neighbors in the cluster). Then we label every other atom in the cluster by its valence minus two. Then, beginning at the origin, we trace a counterclockwise path around the cluster as shown and classify the cluster by its n labels, ordered according to their first appearance along this path. For example, the 3-cluster of Fig. 3 is of class 3, 1, -1, -1, 0, -1, -1. As a further example, the circled atom in Fig. 2 is part of a 2-cluster of class 3, 1, -1, 1, -1, -1, 2, -1, -1, -1, 0, -1. In general the class of a cluster of size n is given by a sequence of n integers $x_0, x_1, ..., x_{n-1}$, with $0 \leqslant x_0 \leqslant z$, and $-1 \leqslant x_i \leqslant z - 2$, for $i > 0$.

The purpose of defining the labels in this way is that the cluster classes then have the property that all of the partial sums of each sequence are positive, while the full sum is zero,

$$S(j) = \sum_{i=0}^{j} x_i \begin{cases} > 0 & \text{for all } j < n - 1 \\ = 0 & \text{for } j = n - 1 \end{cases} \tag{1}$$

As a result we will find that we can consider the partial sums $S(j)$ as executing a kind of random walk on the integers which begins at the origin with a step of x_0 units along the positive direction, continues with the positive and negative steps of size x_i, and terminates when the random walk first returns to the origin.

In order to calculate the probability distribution for an occupied site being in an m-cluster of size n, we note that each cluster class (each allowed sequence) represents exactly

$$\binom{z}{x_0} \prod_{i=1}^{n-1} \binom{z-1}{x_i+1} \tag{2}$$

distinct clusters, where each factor in the product corresponds to the different choices of which neighbors of each cluster site are occupied.

Second, we calculate the probability $P'(\{x_i\})$ that an occupied site is in a *particular* m-cluster of class $[x_0, x_1,..., x_{n-1}]$. As a first step, we write the probability $P'([0])$ that the occupied site is the only site in the m-cluster. This is clearly

$$P'([0]) = \sum_{k=m}^{z} \binom{z}{k} [p(1-r)]^k (1-p)^{z-k} \tag{3}$$

where

$$r = \sum_{l=m-1}^{z-1} \binom{z-1}{l} p^l (1-p)^{z-1-l} \tag{4}$$

is the probability that an occupied neighbor has at least m occupied neighbors of its own and is thus also in the cluster. With this simple example, it is now clear that $P'(\{x_i\})$ is given by

$$P'(\{x_i\}) = p^{x_0} r^{x_0} \sum_{k=\max(0,m-x_0)}^{z-x_0} \binom{z-x_0}{k} [p(1-r)]^k (1-p)^{z-x_0-k}$$

$$\times \prod_{j=1}^{n-1} \left\{ p^{x_j+1} r^{x_j} \sum_{k'=\max(0,m-2-x_j)}^{z-2-x_j} \binom{z-2-x_j}{k'} \right.$$

$$\left. \times [p(1-r)]^{k'} (1-p)^{z-2-x_j-k'} \right\} \tag{5}$$

Third, by combining Eqs. (2) and (5), we formally obtain the probability $P_m(n, p)$ that, at concentration p, an occupied site is in an m-cluster of size n,

$$P_m(n, p) = \sum_{\{x_i\}_n} \binom{z}{x_0} p^{x_0} r^{x_0} \sum_{k=\max(0,m-x_0)}^{z-x_0} \binom{z-x_0}{k} [p(1-r)]^k (1-p)^{z-x_0-k}$$

$$\times \prod_{j=1}^{n-1} \binom{z-1}{x_j+1} p^{x_j+1} r^{x_j} \sum_{k'=\max(0,m-2-x_j)}^{z-2-x_j} \binom{z-2-x_j}{k'}$$

$$\times [p(1-r)]^{k'} (1-p)^{z-2-x_j-k'} \tag{6}$$

where $\sum_{\{x_i\}_n}$ is the sum over all classes of n site clusters [or sequences of n numbers satisfying Eq. (1)].

Finally, this expression (6) can now be viewed as a random walk of $S(j)$ on the integers with the step probabilities

$$P_l = \binom{z-1}{l+1} p^{l+1} r^l \sum_{k=\max(0,m-2-l)}^{z-2-l} \binom{z-2-l}{k} [p(1-r)]^k (1-p)^{z-2-l-k}$$

(7)

for $l = -1, 0,..., z - 2$, of a step being one of l units to the right (of course, $l = -1$ represents a unit step to the left). Then, we find

$$P_m(n, p) = \sum_{\{x_i\}_n} \binom{z}{x_0} \binom{z-1}{x_0-1}^{-1} pr^2 P_{x_0-2} \prod_{j=1}^{n-1} P_{x_j}$$

(8)

But this sum can be written as

$$P_m(n, p) = \sum_{x_0=m}^{z} \binom{z}{x_0} \binom{z-1}{x_0-1}^{-1} pr^2 P_{x_0-2} Q_{x_0}(n-1)$$

(9)

for $n > 1$, where $Q_{x_0}(n - 1)$ is the probability that a random walk defined by the step probabilities P_l, starting at the point x_0 units to the right of zero, first visits zero on the $(n - 1)$th step. Thus, the problem of calculating $P_m(n, p)$ is transferred to that of finding Q_{x_0}. But the random walk problem has previously been studied in detail,[9,10] so that the relevant properties of Q_{x_0} are known.

Since the random walk defined above has negative steps of only one size (-1), it is a "left continuous" random walk, for which it is known (see Ref. 9, Chapter 7) that $Q_x(n)$ is given by

$$Q_x(n) = (x/n) P_{-x}^{(n)}$$

(10)

where $P_{-x}^{(n)}$ is the probability that after n steps, the position will be x steps to the left. These quantities are related to the $\{P_l\}$ as the $(-x)$th moment of their generating function,

$$\psi(y) = \sum_{l=-1}^{z-2} P_l y^l$$

(11)

raised to the nth power. That is, the $P_l^{(n)}$ are defined by

$$\psi^n(y) = \sum_l P_l^{(n)} y^l$$

(12)

From the definition (11) it is clear that, since the P_l are normalized, $\psi(1) = 1$. Furthermore, from Eq. (11), we have that the critical concentration p_c is that concentration for which

$$\langle l \rangle_{p_c} = \frac{d\psi(y)}{dy}\bigg|_{y=1} = 0$$

(13)

since the infinite cluster is here associated with a walk that never returns to zero, and when it first occurs the average step is neither to the left (which causes finite clusters) nor to the right[9,10] (which causes the infinite cluster occupying a nonzero fraction of the lattice).

Finally, to obtain the generating function for the cluster size distribution, we consider $\zeta(t)$, the lowest real root of

$$t\psi(y) = 1 \tag{14}$$

Since the P_l are normalized to one, Eq. (11) gives that there is always a root of Eq. (14) at $y = 1$, $t = 1$. But $\psi(y)$ is a polynomial in y plus a positive term proportional to y^{-1}; thus, it is clear that

$$\zeta(1) = \begin{cases} = 1 & \text{for} \quad \psi'(1) \leqslant 0 \\ < 1 & \text{for} \quad \psi'(1) > 0 \end{cases} \tag{15}$$

so that the critical concentration p_c is that point where the root $\zeta(1)$ reaches one. Finally, we note (see Ref. 9) that for left continuous random walks $\zeta(t)$ is a generating function for the Q_x according to the relation

$$\sum_{n=0}^{\infty} Q_x(n)t^n = \zeta^x(t), \quad \text{for} \quad 0 < |t| < 1 \tag{16}$$

We are now ready to calculate explicitly the relevant properties for the Bethe lattice. First, we use the specific form (7) for P_l, and Eq. (11) to calculate $\psi(y)$, namely,

$$\psi(y) = \frac{1}{yr} \sum_{l=-1}^{z-2} \binom{z-1}{l+1} (yrp)^{l+1} \sum_{k=\max(0,m-2-l)}^{z-2-l} \binom{z-2-l}{k}$$
$$\times [p(1-r)]^k (1-p)^{z-2-l-k} \tag{17}$$

which after some manipulation becomes the simpler form

$$\psi(y) = \frac{1}{yr} \sum_{k=m-1}^{z-1} \frac{z-1}{k} \{p[1-r(1-y)]\}^k (1-p)^{z-1-k} \tag{18}$$

which is also a useful form for $y \approx 1$.

Thus, the critical concentration is easily evaluated as [see Eq. (13)] that concentration where $d\psi(y)/dy = 0$, or the solution of the equation

$$1 = \sum_{k=m-1}^{z-1} k \binom{z-1}{k} p_c{}^k (1-p_c)^{z-1-k} \tag{19}$$

This result is especially simple in the two extreme cases $m = 1$ or 2, and $m = z$, where we find
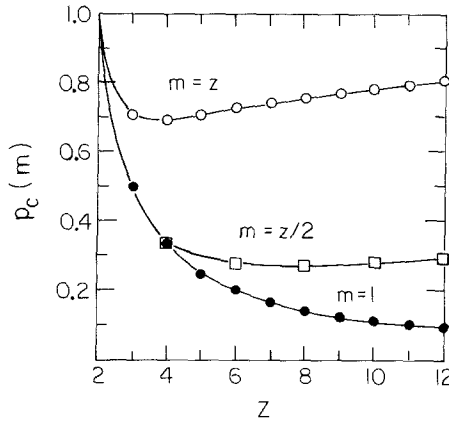
$$p_c(m = 1, 2) = 1/(z-1) \tag{20}$$

Fig. 4. The critical percolation concentration vs. z, for $m = 1$, $z/2$, and z; the limiting values of $p_c(z)$ as $z \to \infty$ are 0, 1/2, and 1 in these cases, respectively.

in agreement with the ordinary percolation result, and

$$p_c(m = z) = [1/(z - 1)]^{1/(z-1)} \tag{21}$$

The fact that $p_c(2) = p_c(1)$ follows from the fact that the infinite 1-cluster contains an infinite 2-cluster. These results and the case $m = z/2$ are illustrated in Fig. 4. For the case $m = m(z)$ it is clear that the limit $z \to \infty$ is characterized by

$$\lim_{z \to \infty} p_c(m(z)) = \lim_{z \to \infty} [m(z)/z] \tag{22}$$

since with an infinite number of near neighbors at concentration p, the fraction p will always be occupied. It seems that for the case where $m = \alpha z$ a minimum value of $p_c(m(z))$ vs. z appears. For $m = z$, according to Eq. (21), this minimum occurs at $z = 1 + e$.

With similar algebra we can, using Eqs. (7), (9), and (16), write the generating function for the cluster size distribution,

$$G(p, t) = \sum_{n=0}^{\infty} P_m(n, p)t^n$$

$$= P_m(0, p) + t \sum_{x_0 = 0}^{z} \binom{z}{x_0} [\zeta(t)pr]^{x_0} \sum_{k = \max(0, m - x_0)}^{z - x_0} \binom{z - x_0}{k}$$

$$\times [p(1 - r)]^k (1 - p)^{z - x_0 - k} \tag{23}$$

This formula can be simplified somewhat to

$$G(p, t) = (1 - p)^z \left(\sum_{k=0}^{m-1} \binom{z}{k} \left(\frac{p}{1 - p} \right)^k \right.$$

$$\left. + t \sum_{k=m}^{z} \binom{z}{k} \left(\frac{p}{1 - p} \right)^k \{1 - [1 - \zeta(t)]r\}^k \right) \tag{24}$$
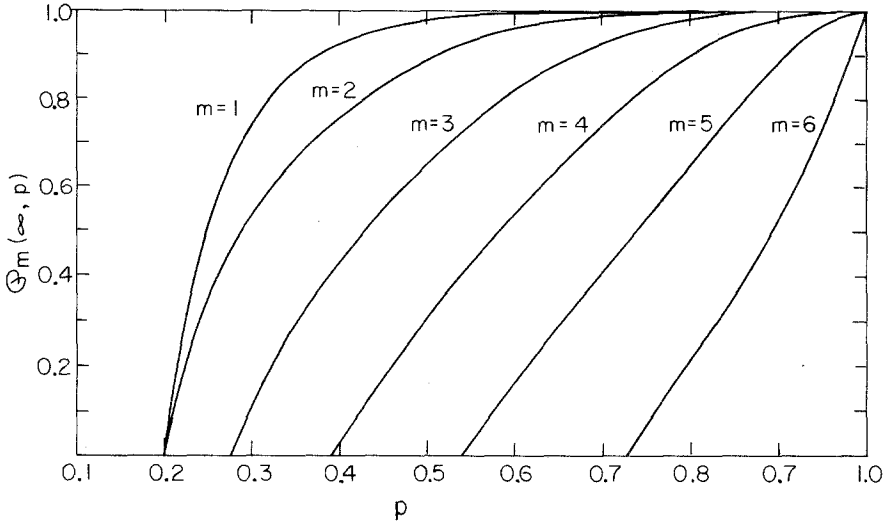
Fig. 5. The percolation probability $P_m(\infty, p)$ vs. p for all values of m with $z = 6$ on the Bethe lattice.

which can easily be evaluated numerically for arbitrary m and z, and studied analytically in various limiting cases. In particular, we consider the probability of finding an occupied site in an infinite cluster

$$P_m(\infty, p) = 1 - \sum_{n=0}^{\infty} P_m(n, p) = 1 - G(p, 1) \qquad (25)$$

and the mean size of the finite clusters

$$\langle n \rangle_{\text{finite}} = \sum_{n=0}^{\infty} n P_m(n, p) = \frac{\partial G(p, t)}{\partial t}\bigg|_{t=1} \qquad (26)$$

These two quantities have been evaluated numerically from Eq. (24) and are shown in Figs. 5 and 6 for all values of m with $z = 6$. We note that, from Eqs. (15) and (24), the percolation probability $P_m(\infty, p) \equiv 0$, for all $p \leqslant p_c$. From these results it is clear that all values of m generally produce qualitatively similar behavior to that of ordinary percolation ($m = 1$) on the Bethe lattice. One exception is that $P_{m=z}(\infty, p)$ approaches one as $p \to 1$ with finite slope when $m = z$, since, the number of occupied sites removed from the infinite cluster is, for small $1 - p$, proportional to $1 - p$ the number of vacancies.

The critical exponents β and γ are determined by the power law singularities in $p - p_c$ of Eqs. (25) and (26) at $p = p_c$. To evaluate the exponent β we first determine the behavior of $\zeta(1)$ for p near p_c, with $\psi(\zeta)$ determined
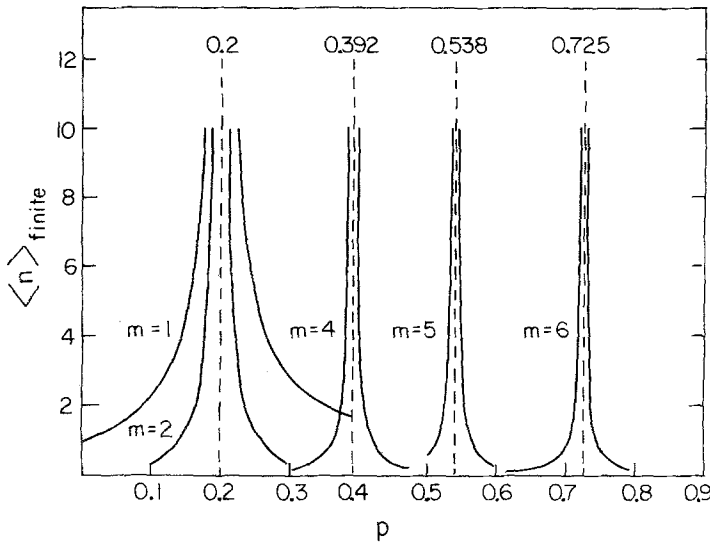
Fig. 6. The mean size of finite clusters $\langle n \rangle_{\text{finite}}$ vs. p for $m = 1, 2, 4, 5$, and 6 with $z = 6$ on the Bethe lattice.

by Eq. (18). For small $p - p_c$, this root occurs at $\zeta(1) \equiv 1 - 2\psi'(1)/\psi''(1)$, which can be shown to be given by

$$\zeta(1) \approx 1 - a_1'(p_c)[r(p_c)a_2(p_c)]^{-1}(p - p_c) + O(p - p_c)^2$$
$$= 1 - A(p - p_c) + O(p - p_c)^2 \tag{27}$$

where

$$a_j(p) = \sum_{k=m-1}^{z-1} \binom{k}{j}\binom{z-1}{k} p^k(1-p)^{z-1-k} \tag{28}$$

Thus, we find

$$\zeta(1) = \begin{cases} 1 & \text{for} \quad p < p_c \\ 1 - A(p - p_c) & \text{for} \quad p \geqslant p_c \end{cases} \tag{29}$$

so that, by Eqs. (24) and (25),

$$P_m(\infty, p) = \begin{cases} 0 & \text{for} \quad p \leqslant p_c \\ zAp_cr^2(p_c)(p_c - p) & \text{for} \quad p \geqslant p_c \end{cases} \tag{30}$$

and $\beta = 1$ for all m. To obtain the exponent γ we similarly evaluate $\zeta'(1) = -1/\psi'(1) = +[a_1'(p_c)(p_c - p)]^{-1}$, which with Eqs. (24) and (26) gives $\langle n \rangle_{\text{finite}} \sim (p_c - p)^{-1}$ for p near p_c or gives $\gamma = 1$, for all m. Thus the Bethe lattice and mean field values of the critical exponents for high-density percolation are the classical[2,11] values $\beta = \gamma = 1$.

Finally, we evaluate the asymptotic form for large n of the cluster size distribution. This form can be obtained directly from Eq. (24), but a physically clearer derivation is as follows. First, we recall[3] that in general the probability $P(n, b)$ that an occupied site is in a cluster of n occupied sites which is surrounded by b vacant perimeter sites in the ordinary ($m = 1$) percolation problem is given by

$$P_1(n, b) = M(n, b)p^{n-1}(1 - p)^b \tag{31}$$

where $M(n, b)$ is the number of such distinct clusters that can be drawn about the site. Then for ordinary percolation on a Bethe lattice it follows that[3,12] $P(n)$ is, for large n, of the asymptotic form

$$P_1(n) = \sum_b P_1(n, b) \underset{n \to \infty}{\sim} \frac{A}{n^{3/2}} \exp[-a(p)n] \tag{32}$$

where $a(p)$ vanishes at $p = p_c$ as $(p_c - p)^2$.

Next, we consider z-cluster percolation. Here it is useful to consider the probability $P_z(n, b)$ that an occupied site is in a cluster of n occupied sites surrounded by b occupied sites (each of which is itself not completely surrounded by occupied sites). On a Bethe lattice this quantity is clearly

$$P_z(n, b) = M(n, b)p^{n-1}[p(1 - p^{z-1})]^b \tag{33}$$

where $M(n, b)$ is the same quantity as that in Eq. (31). But, since $b = (z - 2)n + 2$ on Cayley trees, this equation becomes

$$P_z(n, b) = pM(n, b)(p^{z-1})^n(1 - p^{z-1})^b \tag{34}$$

Therefore, clearly p^{z-1} plays the role for $m = z$ that p plays for $m = 1$. This makes clear the reason for the respective p_c values in Eqs. (20) and (21). But, in addition, it is clear that asymptotically $P_z(n)$ also obeys a form similar to Eq. (32), namely

$$P_z(n) = \sum_b P_z(n, b) \underset{n \to \infty}{\sim} \frac{B}{n^{3/2}} \exp[-a'(p)n] \tag{35}$$

Finally, we note that $P_m(n)$ for $1 < m < z$ must be sandwiched between the values for $m = 1$ and $m = z$, so that its asymptotic form must also be exponential with n as in Eq. (35).

In conclusion, we have demonstrated that m-cluster percolation on a Bethe lattice is similar in all important aspects for all values of m and z. However, it may be that, on a real d-dimensional lattice where closed loops exist, high-density percolation has different exponents from those of ordinary percolation. In any case, we expect the mean-field values of the exponents to be $\beta = \gamma = 1$ independent of m.

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