Percolation and conductivity: A computer study. I*

G. E. Pike and C. H. Seager
Sandia Laboratories, Albuquerque, New Mexico 87115
(Received 7 September 1973)

In this paper and its sequel we consider the relation between various conductivity problems and their associated percolation models. The emphasis of this paper is on the methods of solving percolation problems. Toward that end we define the percolation problem and propose a classification for several types of models. This classification scheme is useful for regular and random lattices and shows the connection between bond and site percolation models. With the aid of a large computer we have used Monte Carlo techniques to solve many random-lattice percolation models in two and three dimensions. These models illustrate the effects of hard-core interactions between sites, of deterministic and probabilistic bonding parameters, and of changing the functional form of the bonding criterion. The random-lattice solutions are used to examine the critical volume fraction concept and the critical number of bonds per site (B_c) concept. These concepts have been previously proposed as methods of obtaining solutions to percolation problems. We find that, subject to several conditions, these concepts may be used for approximate solutions.

I. INTRODUCTION

The use of percolation theory[1,2] to solve physical problems involves two basic steps. First, the physical situation must be simulated by an appropriate percolation model, if one exists. These percolation models are composed of *sites* and of *bonds* between sites (vertices and edges in the nomenclature of graph theory). In general their relation to physical problems is made by identifying the site with sources of interaction and the bonds with interactions of some minimum strength or greater. As a second step then, the properties of this percolation model must be determined. In this paper we characterize several different kinds of percolation models. The emphasis here is on the mathematical concepts and considerations needed to solve the percolation problems. Several simple examples are given. In the following paper[3] (hereafter referred to as paper II) we address the questions of how and when percolation models may be advantageously used to solve physical problems. As detailed examples we compute the electrical conductivity of several model materials, including some which simulate impurity conduction in crystalline semiconductors and variable-range hopping in amorphous semiconductors. These calculations are performed by a Monte Carlo technique with the aid of a computer and the results are compared to the predictions of percolation theory.

Before discussing the details of specific percolation problems, we use Sec. II of this paper to formally develop several concepts concerning percolation. These features are then used to define a classification scheme for percolation models of various types. Section III contains a discussion of primary methods for solving percolation problems. In particular, a description of our Monte Carlo technique is included. In Sec. IV we present results of Monte Carlo solutions to many percolation problems. On the basis of these results we examine in Sec. V the validity of empirical "rules of thumb" which others have used to solve percolation problems; these are the critical volume fraction rule[4] and the average number of bonds per site rule.[1,5] We show that as general rules they certainly fail, but for certain classes of problems they may be quite useful as accurate approximations. Our results are summarized in Sec. VI.

II. DEFINITION OF THE PERCOLATION PROBLEM

Before discussing the solutions of specific percolation problems, we wish to set forth our views concerning the types of problems to be solved. We do this to establish a framework in which relations between problem types may be seen, and also because conventional, regular lattice model classifications are not sufficiently general to describe problems on the random lattice. For readers who are familiar with previous discussions of percolation on regular lattices, we note that although our formulation may seem at first quite different, it is equivalent to the others in all essential aspects. It is only necessary to remember that in our formulation the term "site" is the same as an "occupied site" in previous work.[1,2]

The essence of percolation theory is to determine how a given set of sites, regularly or randomly positioned in some space, is interconnected. Although percolation theory may be applied to finite sets, we consider only the case for which we have a given infinite set of sites. This set extends infinitely far in one or more dimensions. To determine how these sites are interconnected we need the *bonding criterion* which specifies whether

any two sites are connected. (The bonding criterion could involve more than two sites, but we shall consider only pairwise criteria.) The bonding criterion is in general a function of one or more *bonding parameters*. These parameters may or may not be directly associated with the sites. In the former case they are *deterministic* parameters, in the latter they are *probabilistic* parameters. Two sites belong to the same *cluster* if there is an unbroken sequence of bonds from the first site, through other sites, to the second site. For a given set of sites, percolation theory attempts to determine the distribution of cluster sizes as a function of the bonding criterion. In particular, and of primary interest in this paper, one would like to find the bonding criterion for which clusters of infinite size first form.

The bonding criteria of interest to us may always be expressed by a *bonding function*, B_{ij}, which is a Heaviside (step) function,

$$H(x) = \begin{cases} 0 & \text{if } x < 0 \\ 1 & \text{if } x \geq 0 \end{cases},$$

or a product of such functions. The argument of each $H(x)$ is an expression of the form

$$x = C - F_{ij}(\{\delta_i, \delta_j\}, \{p_{ij}\}),$$

where $\{\delta_i, \delta_j\}$ represents the set of deterministic parameters assigned to sites i and j, $\{p_{ij}\}$ is the set of probabilistic parameters for the ij pair, F_{ij} is some function of these parameters, and the quantity C we shall call the *cluster parameter*, since its value determines the distribution of cluster sizes in a given model. Formally, we say that a bond between sites i and j exists if and only if

$$B_{ij} = \prod_{a=1}^{A} H_a(C_a - F_{a,ij}) = 1 , \tag{1}$$

where A is the number of Heaviside functions in the bonding criterion.

We shall find it convenient to classify all types of percolation models according to their bonding criteria in the following manner: (i) If the bonding criterion contains *any* probabilistic parameters, it is a *probabilistic bond* model. (ii) If all bonding parameters are deterministic, and if the number of independent parameters, n, is less than or equal to the dimensionality of the space in which we choose to treat the model, then it is a *site* model in n-dimensional space; otherwise it is a *deterministic bond* model.

Within our classification scheme, we note that site percolation becomes merely a special case of bond percolation.[6]

III. PRIMARY METHODS OF PERCOLATION SOLUTIONS

Before examining the solutions of various bond and site percolation problems, we first want to consider the methods of solving these problems. A complete solution would entail establishing the entire distribution of cluster sizes as a function of the bonding parameters and bonding criterion. Such a complete solution is beyond the scope of this paper and we confine ourselves here to the determination of the critical value of the cluster parameter, C_c; i.e., the value at which infinite clusters first form. As we show in paper II, this is the quantity used in the critical path analysis of physical problems and thus is important by itself.

A. Exact methods

Only for a few special cases have exact solutions to percolation problems been obtained. Fisher and Essam[7,8] have obtained several exact results for percolation on Cayley trees and related cacti. A Cayley tree is a lattice for which a closed loop of sequential bonds is forbidden and a cactus is obtained by decorating the vertices of trees with finite graphs. Also by taking advantage of special properties of certain two-dimensional regular lattices with nearest-neighbor bonding, Sykes and Essam[9] have deduced exact solutions for a few cases. These solutions have been marked by a superscript e in Table I.

Aside from those just mentioned, we know of no other exact solutions to percolation problems. That is, no exact results at all are available for three or more dimensions. Even in two dimensions none is available for random lattices, for nth ($n > 1$) nearest-neighbor bonding, for zero hard-core size, or for correlation effects. Although Zallen and Scher[10] have recently proposed an exact solution for a special case of "percolation on a continuum," we shall demonstrate by counterexample in Appendix A that their claim is unwarranted.

B. Approximate methods

In lieu of exact results, two primary methods of estimating percolation solutions to specific problems have been used extensively. By forming a series expansion of the mean cluster size, one may study the convergence properties of this series as a function of the bonding parameters and the bonding criterion.[11] We shall not discuss this technique further. The other technique is to utilize Monte Carlo methods in conjunction with a large computer.[12,13] This is how we have obtained all our results presented here.

Because most of the physical problems in which we were interested involve random site positions, and because we felt that regular lattice cases had already been adequately (for our present purposes) solved by others,[1] we have solved only percolation models with random site placement. For purposes of later discussion, however, we summarize many

TABLE I. Percolation results for regular lattices.[a] A superscript *e* indicates an exact result from Refs. 7 and 11. In the column headings n denotes bonding out to the nth nearest neighbor, z is the total coordination number corresponding to n, f is the packing fraction of spheres, $p_{s,c}$ is the critical site percolation probability, $p_{b,c}$ is the critical bond percolation probability, CVF is the critical volume fraction (Ref. 4), and $\bar{B}_c$ is the average number of bonds per site at percolation.

Lattice	n	z	f	$p_{s,c}$	CVF $fp_{s,c}$	$\bar{B}_c$ $zp_{s,c}$	$p_{b,c}$	$\bar{B}_c$ $zp_{b,c}$
Honeycomb	1	3	0.61	0.700	0.427	2.10	0.6527^e	1.96^e
	3	12	•••	0.300	•••	3.60		
Kagomé	1	4	0.68	0.6527^e	0.444^e	2.61^e		
Square	1	4	0.79	0.590	0.466	2.36	0.5000^e	2.00^e
	2	8	•••	0.410	0.548	3.28		
	3	12	•••	0.292	•••	3.50		
Triangular	1	6	0.91	0.500^e	0.455^e	3.00^e	0.3473^e	2.08^e
	2	12	•••	0.295	•••	3.54		
	3	18	•••	0.225	•••	4.05		
Diamond	1	4	0.34	0.425	0.145	1.70	0.388	1.55
sc	1	6	0.52	0.307	0.160	1.84	0.247	1.48
	2	18	•••	0.137	0.192	2.47	•••	•••
	3	26	•••	0.097	•••	2.52		
bcc	1	8	0.68	0.243	0.165	1.94	0.178	1.42
	2	14	•••	0.175	•••	2.45		
	3	26	•••	0.095	•••	2.47		
fcc	1	12	0.74	0.195	0.144	2.34	0.119	1.43
	2	18	•••	0.136	•••	2.45		
	3	42	•••	0.061	•••	2.56		
hcp	1	12	0.74	0.204	0.151	2.45	0.124	1.49

[a]After Shante and Kirkpatrick (Ref. 1).

regular lattice results[1] in Table I.

Since our Monte Carlo method of solving percolation models differs somewhat from previously published ones, we give a brief description of our technique. Using the RANF pseudorandom number generator available on PDP-10 and the CDC-6600 computer systems, we generate the site coordinates and any of the other bonding parameters. On both computers the output of RANF is a number between zero and one. The PDP-10 returns this number with 27 binary bits (8 significant decimal places), while on the CDC-6600 the number has 48 binary bits (roughly 14 significant decimal places). The starting points or "seeds" for RANF were selected for each computation by generating then discarding a selected, but arbitrary, number of unused numbers. To generate the coordinates for N sites we picked a seed, generated all N of the x_i, picked another seed, generated all of the y_i, and likewise for z_i (if used). This procedure produces a random array of N_s sites in a square (cube) of side unity and thus the site density is also given by N_s. If additional bonding parameters were assigned, RANF was used in the same way.

For a given bonding criterion every site is checked against every other site. If two sites satisfy the bonding criterion, they are assigned a common cluster identification number. All sites within the same cluster have the same cluster identification number

To test for percolation we establish *boundary regions* at the edges of the squares (cubes) as illustrated in Fig. 1. Their thickness is roughly the critical bonding distance. If any two sites in opposite boundary regions have the same cluster identification number, then we say the sample is percolating in the direction perpendicular to that boundary.

For a given sample we start with a subcritical value C for the cluster parameter and check for percolation. The value of C is increased in small increments until percolation is detected in all spacial dimensions. We take the critical value C_c of the cluster parameter to be the average of the C_c values for each direction of percolation. For each percolation model considered we have run many different samples. The average of all determined C_c for a given model and the standard deviation of their distribution were computed. For models in which C_c is a critical bonding radius R_c,

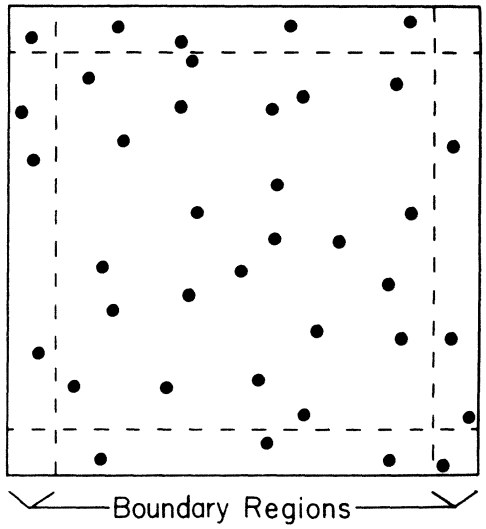

FIG. 1. Illustration of boundary regions used in our method of solution. When sites in opposite boundary regions first belong to the same cluster, we say that the sample is percolating in that direction.

the results are given in column 6 of Tables II and III. All of our results are presented in detail in the next section.

IV. RANDOM-LATTICE RESULTS

Using our Monte Carlo parameter selection technique we have solved various percolation models. The results, in terms of the critical cluster parameter value, are given here and summarized in Tables II and III. The motivation for our choice of models and the implication of the results are discussed in Sec. V.

A. Circles

Within this section we describe our solutions to several two-dimensional models in which bonding is wholly or partly determined by the distance between sites. That is, the bonding function will contain $H[R - F_{ij}(d_{ij})]$, where $F_{ij}(d_{ij})$ is some function of the intersite separation

$$d_{ij} = [(x_i - x_j)^2 + (y_i - y_j)^2]^{1/2} .$$

For purposes of latter discussion, both here and in paper II, it is helpful to visualize these models (and others) in terms of two, geometric constructions. As a specific illustration of these, we consider site percolation on the random two-dimensional lattice for which the bonding criterion is,

$$B_{ij} = H(R - d_{ij}) = 1 . \qquad (2)$$

The left-hand side of Fig. 2 shows what we shall call the *inclusive figure* (IF) construction. About each site a circle of radius R is drawn. By Eq. (2) two sites lying within each other's circle are bonded; otherwise they are not. The percolation problem is to find the critical radius R_c at which an infinite cluster of connected sites is formed. The second geometric construction, which historically has been used much more often than the IF, is illustrated for this model in the right-hand half of Fig. 2. Again, circles of some radius r ($=\frac{1}{2}R$) are circumscribed about each site. However in this construction, two sites are bonded if their associated circles overlap. We shall call this the *overlapping figure* (OLF) construction. Although the IF and OLF constructions are trivially related for this percolation problem, we have presented them for a definite purpose. Using OLF constructions (mainly on regular lattices) workers have used critical volume fraction methods to solve percolation problems.[4,10,14–16] In Sec. V of this paper we examine this method, as originally proposed, and find it to be a bad approximation in many cases. On the other hand, the IF construction is more general and is better suited to demonstrating the relation between site and bond percolation problems on both regular and random lattices.

With these two types of construction in mind, we now consider the site and two types of bond models on the two-dimensional random lattice for sites with no hard-core interaction. That is, sites may

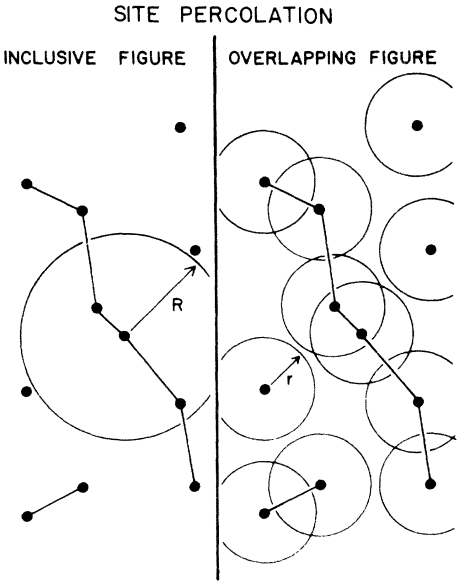

FIG. 2. Illustration of inclusive figure and overlapping figure constructions for two-dimensional random-lattice site problem. The same set of randomly located sites is shown in each half of the figure. All bonds between sites whose separation is less than or equal to R ($=2r$) are drawn. For clarity only the IF circle about the central site is shown although all sites have one in the IF construction.

TABLE II. Percolation results for the random two-dimensional lattice. r_{HC} is the hard-core radius, $\bar{r}_s = 1/\sqrt{\pi N_s}$, p_b is the probabilistic bond probability, N_s is the site density, the number of computer samples solved for each model is shown to the right of N_s, R_c is the critical bonding radius at percolation, σ_R is the standard deviation of the data used to find $R_c/2\bar{r}_s$, $\bar{B}_c$ is the average number of bonds per site at percolation, and CAF is the critical area fraction.

Model Shape	$r_{HC}/\bar{r}_s$	p_b	N_s	No. of samples	$R_c/2\bar{r}_s$	σ_R	$\bar{B}_c$	CAF
Uniform circles	0	1	400	12	1.064	0.058	4.53	0.678
	0	1	1000	23	1.067	0.037	4.55	0.680
	0	1	4000	13	1.058	0.026	4.48	0.674
	0.3	1	1000	22	0.996	0.042	3.57	•••
	0.5	1	1000	22	0.923	0.020	2.68	•••
	0.707	1	1000	22	0.887	0.009	2.16	•••
	0.707	1	400	8	0.898	0.009	2.30	•••
	0	0.50	4000	20	1.28	•••	3.28	•••
	0	0.25	4000	20	1.585	•••	2.51	•••
Variable circles $r_i = E_i R_c/2$, $1 \geq E_i \geq 0$	0	1	1000	18	1.853	0.088	4.01	0.682[a]
	0	1	4000	16	1.848	0.053	3.98	0.680
Uniform squares	0	1	4000	8	1.050[b]	0.023	4.41	0.668
Sticks random angle	0	1	1000	10	2.118	0.045	3.635	0

[a]See Appendix B.

[b]Equivalent-area circle radius. See Sec. IV B of text.

lie arbitrarily close together. Then the effect of having a hard core is examined. In all cases the critical radius will be normalized by $2\bar{r}_s \equiv 2/\sqrt{\pi N_s}$. This is an arbitrary, but convenient, normalization factor which is roughly the average lattice constant for these random lattices.

1. Site percolation

For this site percolation problem all sites within some radius R of another site are bonded to this site as discussed above. In paper II the solution of this model is used directly to calculate impurity conductivity in lightly doped low compensation semiconductors. For samples of $N_s = 400$, 1000, and 4000, we find the average critical radius $R_c/2\bar{r}_s$ to be 1.064, 1.067, and 1.058, respectively. The effect of increasing the sample size by a factor of 10 is mainly to decrease the standard deviation of the distribution of individual sample values. Although the average value changes by less than 1%, there is a tendency (more noticeable in the three-dimensional results) for the small samples to yield larger values for R_c. Ambegaokar, Cochran, and Kurkijärvi[17] have observed a similar behavior in terms of resistor networks which they explain as due to the finite sizes of the samples.

Other investigators have attempted to calculate the value of R_c for this model. Using a Monte Carlo technique Gilbert[18] estimates $R_c/2\bar{r}_s = 0.895$, and by a different Monte Carlo method, Roberts[19] deduces $R_c/2\bar{r}_s = 0.977$. We believe both of these values to be in error because the procedures for obtaining them did not properly account for large clusters.[20,21] Pollak[22] has calculated a lower bound of $R_c/2\bar{r}_s \geq 0.5$ for this problem.[23]

Dalton, Domb, and Sykes[24] have used a series-expansion technique to examine site percolation on

TABLE III. Percolation results for the random three-dimensional lattice. All symbols have the same meaning as in Table II, except that $\bar{r}_s = (3/4\pi N_s)^{1/3}$ and CVF is the critical volume fraction.

Model Shape	$r_{HC}/\bar{r}_s$	p_b	N_s	No. of samples	$R_c/2\bar{r}_s$	σ_R	$\bar{B}_c$	CVF
Uniform spheres	0	1	1000	65	0.7150	0.0229	2.92	0.306
	0	1	8000	13	0.7048	0.0057	2.80	0.295
Variable spheres $r_i = E_i R_c/2$, $1 \geq E_i \geq 0$	0	1	8000	5	1.131	0.004	2.17	0.303[a]

[a]See Appendix B.

many regular lattices as a function of increasing bonding range. Extrapolating the results from first, second, and third nearest-neighbor bonding to much larger bonding distances they find 4.5 bonds per site at percolation. This extrapolated result should yield our results since the effect of the hard core and the regularity of the regular lattice becomes negligible for bonding distances much larger than the hard-core radius.[1] Their value of 4.5 bonds per site corresponds to a critical radius of $R_c/2\bar{r}_s = 1.06$, in excellent agreement with our value of 1.058. In light of the above discussion we feel confident in a value of $R_c/2\bar{r}_s = 1.06 \pm .03$.

2. Probabilistic bond percolation

In this percolation model each possible bond between sites, whose separation is less than the maximum bonding radius, has a probability p_b of existing. Thus the bonding function is

$$B_{ij} = H(R - d_{ij})H(p_b - p_{ij}) ,$$

where p_{ij} is a random number with value between zero and one. For $p_b = 1$ we have the site model just considered. To solve the problem for $p_b < 1$ we started with a site model and then eliminated a fraction, $q = 1 - p_b$, of the bonds at random (cf. Fig. 3). Every time we incremented the maximum bonding radius R, we reestablished all possible bonds. The fraction of bonds, q, was then removed four different random ways.

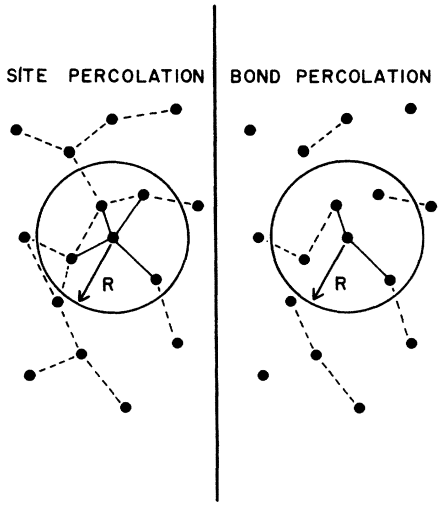

FIG. 3. Illustration of the difference between site and bond percolation models discussed in Sec. IV A. (a) In the site model, bonding is determined solely by the intersite separation, i.e., $B_{ij} = H(R - d_{ij})$. All sites with separations less than or equal to R are bonded. (b) For the bond problems, bonding depends on more than just separation (see text). However, one still has no bonds if $d_{ij} > R$.

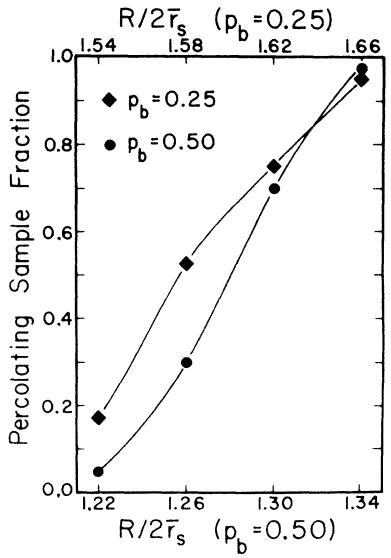

FIG. 4. Fraction of computer samples which percolate versus the reduced bonding radius for the probabilistic bond model. These results pertain to the bond model discussed in Sec. IV A 2. Here an IF circle of radius R is drawn about each site and bonds are made to all other sites within that circle. Then a fraction $q = 1 - p_b$ of these bonds are discarded at random. The fraction of samples which percolate with the remaining bonds is plotted as a function of R. The diamonds and upper abscissa refer to $p_b = 0.25$. The circles and lower abscissa denote results for $p_b = 0.50$.

After each time, we checked for clusters spanning the square. In Fig. 4 we give our results for $p_b = 0.50$ and $p_b = 0.25$. There we plot the fraction of percolating samples versus R. If we determine the critical radius from the value at which this fraction is 0.5, then we find $R_c/2\bar{r}_s = 1.28$ for $p_b = 0.50$ and $R_c/2\bar{r}_s = 1.59$ for $p_b = 0.25$.

3. Deterministic bond percolation

Instead of removing bonds at random, one may make bond elimination dependent on site param-

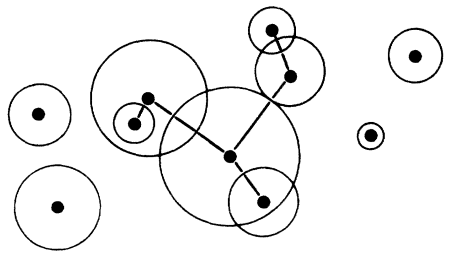

FIG. 5. OLF construction for variable circle (deterministic bond) percolation model. Each site is randomly assigned a parameter E_i between zero and one. The OLF circle about each site has radius $r_i = E_i R/2$. Two sites are bonded if their circles overlap; i.e., if the intersite distance, $d_{ij} \leq (E_i + E_j)R/2$.

eters. One way of doing this is to assign each site a parameter E_i between zero and one. If the bonding function is $B_{ij} = H[R - 2d_{ij}/(E_i + E_j)]$, then again we have a bond problem in two dimensions with respect to R. This problem is best viewed in an OLF construction as shown in Fig. 5. In the problem we solved, the E_i values were uniformly distributed between zero and one and were assigned randomly using the RANF function. The OLF construction is then a mixture of variable-sized circles with radii ranging from 0 to $\frac{1}{2}R$. For samples of $N_s = 1000$ and 4000 we find $R_c/2\bar{r}_s = 1.853$ and 1.848, respectively. Here, again, increasing the sample size has negligible effect on the average, but does significantly decrease the spread of sample values.

This same problem may also be viewed as site percolation model in a limited three-dimensional space by treating the parameter E_i as the additional dimension. The IF construction in Fig. 6 schematically demonstrates the model. The bonding criterion is the same as before. Even though the model is three dimensional, we are only interested in clusters spanning the two spacial dimensions.

We note here that this model is somewhat correlated in the sense that sites of large E_i are generally bonded to more sites than average. An example of an uncorrelated deterministic bond problem is provided by the stick model considered below (Sec. IV C).

4. Site percolation, nonzero hard core

Thus far we have discussed models in which the sites may be arbitrarily close together. What is the effect of establishing a hard-core circle of radius r_{HC} about each site, so that no site is permitted within $2r_{HC}$ of any other site? We solved this problem for a range of r_{HC}. To do so our site coordinate selection procedure was modified such that first a trial pair of (x_i, y_i) were generated. The computer then checked the distance from this site to all sites already established. If the trial site was not within $2r_{HC}$ of another site, it was accepted as a new site. Otherwise it was discarded and a new pair of (x_i, y_i) was tried. This procedure was followed until the prechosen N_s number of sites were placed. For $r_{HC} = \bar{r}_s/\sqrt{2}$ typically $25N_s$ trial pairs of site coordinates were required to obtain N_s satisfactory sites. Note that our procedure involves no internal or external influence on the sites other than the hard-core exclusion. In particular, no established sites were nudged aside to make room for a trial site. Thus, physically speaking, our samples were not subject to an external compacting force.

As before, the value of the maximum bonding radius was raised until a cluster spanned the square. A graph of our results is shown in Fig. 7. Also shown are results for several regular lattices obtained from the data in Table I.

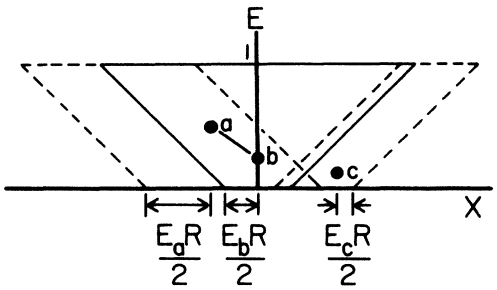

FIG. 6. IF construction for variable circle problem considered as a limited-dimension site percolation model. This construction is for the same problem illustrated by Fig. 5. Only one spatial dimension is shown for clarity. The actual figures are frustrums of right cones whose altitude is unity and whose base radii are $E_iR/2$ and $(1 + E_i)R/2$. In this particular illustration sites a and b are bonded, whereas site c is bonded to neither a nor b.

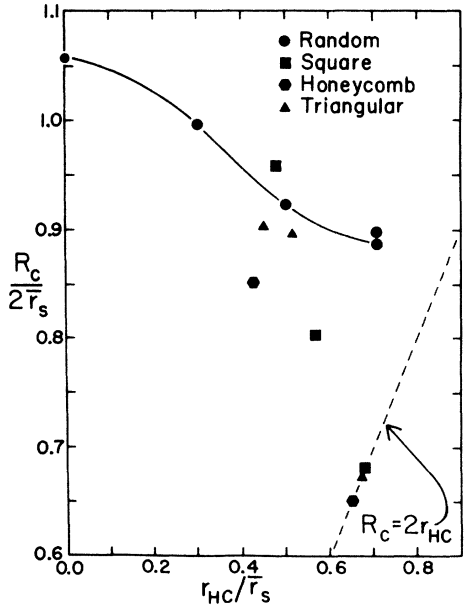

FIG. 7. Effect of a hard core on the critical bonding radius for site percolation in two dimensions. In this graph we plot as circles our Monte Carlo determination of the critical radius R_c as a function of the hard-core radius r_{HC} for site percolation on the random lattice. The upper circle at $r_{HC}/\bar{r}_s = 0.707$ is for the eight samples of 400 sites. The lower circle is the result for the 22 samples of 1000 sites. The solid line is simply a smooth fit to this data. The other points on the graph denote results for site percolation on various regular two-dimensional lattices. The values were determined from Table I. The dashed line is an obvious lower bound to R_c which is exact for regular lattices.

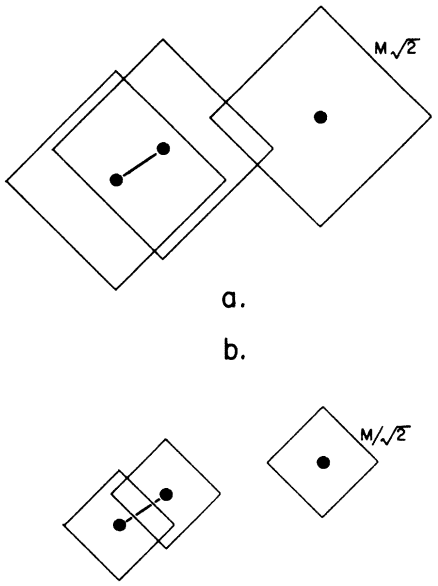

FIG. 8. IF and OLF construction for site percolation model of oriented squares. Part *a* shows the IF and part *b* the OLF constructions for the bonding criterion, $|x_i - x_j| + |y_i - y_j| \leq M$.

B. Squares

Early in our investigation we wondered about the effect of changing the bonding criterion in a site percolation model. Instead of

$$B_{ij} = H\{R - [(x_i - x_j)^2 + (y_i - y_j)^2]^{1/2}\}$$

used for the circles, we chose

$$B_{ij} = H(M - |x_i - x_j| - |y_i - y_j|) .$$

In either an IF or an OLF construction, this criterion yields oriented squares about each site. In the former case the square side is of length $M\sqrt{2}$; in the latter it is $M/\sqrt{2}$ as shown in Fig. 8. Eight samples of $N_s = 4000$ were tested with this criterion. We find the critical value of M to be $M_c/2\bar{r}_s = 1.316$. If one expresses this in terms of the radius of a circle (IF) whose area is equal to the square's area, one finds $R_c/2\bar{r}_s = 1.050$. This is quite close to the value of 1.058 obtained for site percolation with circles.

C. Sticks

Consider a collection of sticks (line segments) of length L, each centered on a site. Each stick is given a random azimuthal orientation, $\pi \geq \theta_i \geq 0$ as shown in Fig. 9. If two sites are bonded when their sticks overlap, what is the stick length required to have percolation? To answer this question we generated ten samples of $N_s = 1000$ in the normal manner. The θ_i were assigned using RANF. For the bonding criterion we required that

$$B_{ij} = H(L - 2A)H(L - 2B) , \tag{3}$$

where

$$A = d_{ij} \left|\sin(\gamma - \theta_j)/\sin(\theta_i - \theta_j)\right| ,$$

$$B = d_{ij} \left|\sin(\gamma - \theta_i)/\sin(\theta_i - \theta_j)\right| ,$$

$$\gamma = \tan^{-1}[(y_i - y_j)/(x_i - x_j)] ,$$

$$d_{ij} = [(x_i - x_j)^2 + (y_i - y_j)^2]^{1/2} .$$

Using the illustration in Fig. 9 plus the law of sines will demonstrate the correctness of this criterion. Clearly there is a maximum bonding radius $R = L$ for this model. We find the critical value to be $R_c/2\bar{r}_s = L_c/2\bar{r}_s = 2.118$. This is approximately twice as large as the value found for site percolation among uniform circles.

D. Spheres

For three spacial dimensions, we solved considerably fewer problems. To obtain statistics comparable to those in two dimensions, $N_{s,3D}$ must be roughly $(N_{s,2D})^{3/2}$ because the measure of finiteness and fluctuations is determined by the average number of sites per box edge length. The computation time goes nearly as N_s^2 for any dimension, and thus the cost climbs rapidly. Fortunately, most of our comments on percolation theory could be illustrated with two-dimensional examples, and only a few three-dimensional solutions were necessary.

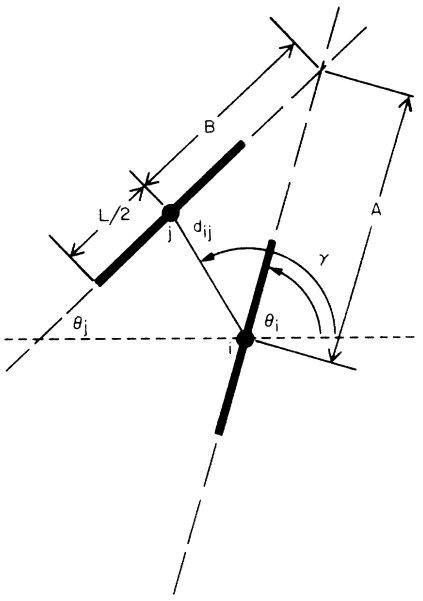

FIG. 9. Diagram for determining bonding criterion for a stick (deterministic bond) percolation model. Each stick of length L is centered on a site and has some randomly assigned orientation angle θ_i. If bonding occurs when two sticks overlap, then the bonding criterion is $A \leq L/2$ and $B \leq L/2$.

1. Site percolation

As in two dimensions, we generated a random array of sites and checked all pairs using the bonding function,

$$B_{ij} = H\{R - [(x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2]^{1/2}\} .$$

Sixty-five of $N_s = 1000$ yielded $R_c/2\bar{r}_s = 0.7150$, where $\bar{r}_s = (3/4\pi N_s)^{1/3}$. For 13 samples of $N_s = 8000$ the value lowered to $R_c/2\bar{r}_s = 0.7048$.

Dalton *et al.*[24] and Domb and Dalton[25] have solved this same problem by their series technique, summarized briefly in Section IV A 1. They find an equivalent critical radius of $R_c/2\bar{r}_s = 0.696$ which is about 1% lower than ours. Because of the observed tendency for the critical value to decrease as the sample size increases, we believe that our value at $N_s = 8000$ may still be somewhat high. In fact an extrapolation of our results versus $(1/N_s)^{1/3}$ yields a limiting value of 0.695.[26]

Roberts and Storey[27] used a Monte Carlo method to solve this problem. From 20 samples with a maximum cluster size of about 25 they attempted an extrapolation to infinite cluster size. Their value was $R_c/2\bar{r}_s = 0.719 \pm 0.006$. However, we do not think their procedure takes proper account of the large cluster sizes.[21] As in two dimensions, Pollak[22] finds a lower bound of $R_c/2\bar{r}_s \geq 0.5$ for this case.[23]

Using site percolation on a simple cubic lattice with the maximum bonding radius equal to three lattice spacings, Holcomb and Rehr[28] obtain a value of $R_c/2\bar{r}_s = 0.66 \pm 0.02$. With their bonding criterion the effects of regularity and the hard core should be negligibly small. We do not understand the difference between their result and ours (but see the comments in Ref. 29).

More recently, Kurkijärvi has estimated $R_c/2r_s$ to be 0.703 from computer calculations of a conductivity problem on the random lattice.[29] Also Skal and Shklovskii[30] using a Monte Carlo program similar to ours have found $R_c/2r_s = 0.721 \pm 0.008$ at $N_s = 1500$, in good agreement with our value of 0.715 at $N_s = 1000$.

2. Deterministic bond percolation

As was shown for two dimensions, we may convert the random site percolation model into a deterministic bond percolation problem by assigning each site a value of E_i, $1 \geq E_i \geq 0$, at random. For site separation d_{ij}, the bonding function is $B_{ij} = H[R - 2d_{ij}/(E_i + E_j)]$. In an OLF construction we have a collection of variable-sized spheres whose individual radii are $r_i = \frac{1}{2}E_i R$. With values of E_i uniformly distributed between zero and one, five samples were solved for $N_s = 8000$. The average critical bonding radius was $R_c/2\bar{r}_s = 1.131$.

Our solutions to all the random-lattice problems discussed above are listed on Tables II and III. We also give in those tables some calculated quantities which will be useful in the next section.

E. Hyperspheres

We have solved one percolation problem involving four spacial dimensions; this is the model of uniform zero-core hyperspheres. The bonding function is

$$B_{ij} = H\{R - [(w_i - w_j)^2 + (x_i - x_j)^2 + (y_i - y_j)^2 + (Z_i - Z_j)^2]^{1/2}\} .$$

We solved three computer samples of $N_s = 10^4$ sites randomly distributed throughout a hypercube. We find that $R_c/2\bar{r}_s = 0.613 \pm 0.068$ where $\bar{r}_s = (2/\pi^2 N_s)^{1/4}$. We do not believe that these three samples are as statistically significant as the small standard deviation might imply. However, we know of no other similar work to which we may compare our result. Although incidental to the main themes of this paper, an interesting relation between the percolation problems of zero-core "spheres" in two, three, and four dimensions is discussed in Appendix C.

V. SECONDARY METHODS OF PERCOLATION SOLUTIONS

For some percolation models, the direct solution by series or Monte Carlo methods can be very difficult. By examining known solutions, theorists have attempted to find common properties of these solutions which might be regarded as invariants. By induction, these "invariants" would be used to determine the critical cluster parameters of unsolved models. In this section we examine two such invariants in some detail.

A. Critical volume fraction

The suggestion has been made,[4] and subsequently widely used,[10,14–16] that the volume fraction occupied by percolating OLF's is an approximate invariant depending only on the dimension of the space. Regular lattice site models with nearest-neighbor bonding (the basis for the original proposal) show quite closely a critical volume fraction (CVF) of 0.15 in three dimensions and a critical area fraction (CAF) of 0.44 in two dimensions.[1,4] However, for more general problems we find that, in addition to the requirement of meaningful OLF constructions, several other considerations must be taken into account when using CVF arguments.

The first point to be recognized is that the CVF depends on the size of the hard core of the OLF's. For the random-lattice hard-core samples that we solved, a calculation of the CVF is very difficult, and so they cannot easily be used to support

this statement. However, Shante and Kirkpatrick[1] have pointed out that the effect can be demonstrated for regular lattices (hard-core radius equal to $\frac{1}{2}$ lattice constant). For example (see Table I), when the maximum bonding radius is changed from first to second nearest neighbor, the CVF for the simple cubic lattice goes from 0.26 to 0.192 and the CAF for the square lattice increases from 0.466 to 0.548. In the limit of bonding to the nth nearest neighbor as $n \to \infty$ regularity of the lattice is negligible, the relative hard-core radius goes to zero, and the problem is equivalent to the zero-core uniform sphere (circle) problem we have solved.[1] The CVF (CAF) is now given by[1] $(1 - e^{-\gamma})$, where γ is the average number of sites within a volume (area) the size of an OLF (the results for our various cases are in column 9 of Tables II and III). As the relative hard-core size decreases to zero, the CVF doubles from 0.15 to 0.295, while the CAF increases from ~0.44 to 0.674. Clearly the CVF and the CAF have a rather strong dependence on hard-core size.

Even among various zero-core site models, the CAF technique yields different values. For example, in Fig. 10 we show a regular hexagon IF. For the bonding criterion this represents, there exist two possible sets of OLF's—equilateral triangles and regular hexagons. The sets are interchangable, since bonds among the two sets are identical. Clearly, though, different areas are involved and the CAF for the hexagons will be near 0.67 found for spheres while the CAF for the triangles will be close to 0.53.

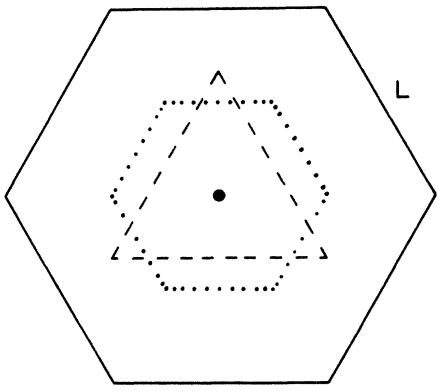

FIG. 10. Illustration of a site model with two different OLF constructions. The solid-line, regular hexagon of side L is the IF for a certain site problem. Either of two alternative sets of OLF's could also be used to represent the bonding criterion: one set consists of regular hexagons of side $L/2$ (dotted line); the other set is equalateral triangles of side L (dashed line). Consider two identical arrangements of sites. Let one set of sites have the hexagons as OLF's and the other have the triangles. Bonding within each set is identical. Thus at percolation the number of bonds per site, $\bar{B}_c$, is the same, but the occupied area fraction, the CAF, is quite different.

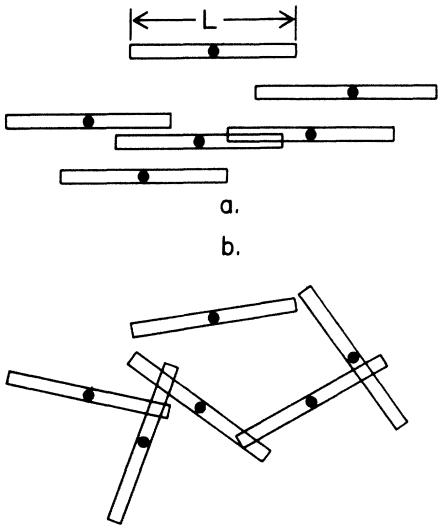

FIG. 11. OLF construction for oriented and unoriented rectangles. Part a illustrates a set of sites on a random lattice; each site is the center of an oriented rectangle of length L. If the width is sufficiently small, no infinite clusters of bonded sites will occur. Part b shows the same sites and rectangles, but now the OLF rectangles have been given an random azimuthal orientation. Regardless of their width if $L \geq 2 \times 2.118\ \bar{r}_s$, the rectangles will form infinite clusters. This figure is to help visualize why the disordered rectangles percolate when an ordered system will not.

To illustrate another condition to be taken into account, consider a randomly placed set of sites which, in an OLF construction, have zero-core oriented rectangles of length $L = 2 \times 2.118 \bar{r}_s$ about them. As shown in Fig. 11(a), let the rectangle width be so small that the occupied area fraction is much less than the zero-core CAF. Thus percolation will not exist. Now let each rectangle assume a random orientation about its site as shown in Fig. 11(b). From our solution to the "stick" model of Sec. IVC, we know that this set of figures will now percolate. In fact, even if the rectangle width went to zero, and hence also the occupied area fraction, the set would still percolate.

Why does the CAF of the oriented rectangle model differ from the CAF of its angularly disordered counterpart? It is not the fact that the latter has an additional random parameter θ_i, nor is it due to the former being a site percolation model while the latter is a bond percolation model; the variable circle and variable sphere models both percolate at the zero-core CVF and thus are counterexamples to each of these hypotheses. The crucial difference, we believe, is in the nature of the bonding criterion. Specifically, it seems that a necessary condition for the validity of the CVF

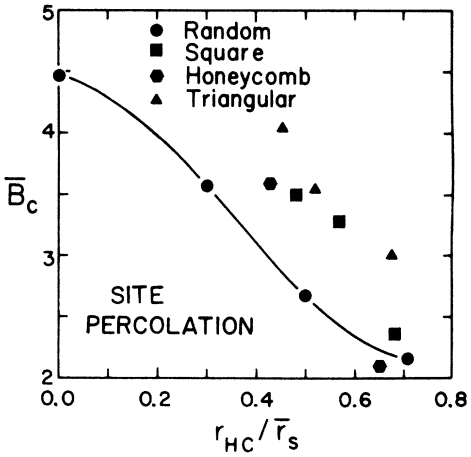

FIG. 12. Effect of a hard core on the critical number of bonds per site. The circles denote our determination of the critical number of bonds per site, $\bar{B}_c$, as a function of hard-core radius r_{HC} for site percolation on a random two-dimensional lattice. The solid line is simply a smooth fit to these points. Also shown for comparison are values for several regular lattices obtained from Table I.

concept is that the bonding function be expressible in the form

$$B_{ij} = \prod_{a=1}^{A} H_a[C_a - M_a(\vec{x}_i - \vec{x}_j)/(f_{a,i}+f_{a,j})] , \qquad (4)$$

where C_a is the cluster parameter for the ath Heaviside function, M_a is a regular function of the spatial coordinates $\vec{x}_i$, and $f_{a,i}$ is a regular function of all other deterministic parameters associated with site i.

Looking at the bonding criterion for the stick problem in Sec. IV C [Eq. (3)] will reveal that it cannot be put into the form of Eq. (4). We want to emphasize that Eq. (4) is a completely empirical condition established on the basis of only a few examples and the authors' intuition. It is probably not sufficient, but it is at lease consistent with the results of all random and regular lattice problems solved to date.

We conclude that the concept of a CVF can provide reasonable, approximate solutions to some percolation problems. However, the CVF values proposed originally[4] must be modified according to the relative hard-core size and other considerations.

B. Average number of bonds per site

Another proposed dimensional invariant is the average number of bonds per site at percolation, $\bar{B}_c$.[1,5] This rule evolved from a study of bond percolation models on regular lattices with nearest-neighbor bonding. Table I, column 9, demonstrates that for these models $\bar{B}_c$ is nearly 2 in two dimensions and nearly 1.5 in three dimensions.

Although this "invariant" may seem topologically more satisfying than the CVF concept, we shall demonstrate that the use of $\bar{B}_c$ also has limited validity. Unlike the CVF rule, the existence of meaningful OLF's is not required to calculate $\bar{B}_c$.

As for the CVF concept, the value of $\bar{B}_c$ depends on the core size relative to the average intersite spacing. This dependence can be seen for regular lattices by examining the $\bar{B}_c$ columns of Table I and the points in Fig. 12. For a given lattice the lowest value of $\bar{B}_c$ occurs for the classical, nearest-neighbor bond model in which the sites are most densely arrayed. Maintaining nearest-neighbor bonding, if the sites are thinned to the classical site percolation density (concurrently increasing the bond probability to unity), then $\bar{B}_c$ increases considerably. As the site density is decreased further (and bonding radius necessarily increased), the value of $\bar{B}_c$ continues to increase. In the limit of bonding radius large compared with the underlying vertex spacing, the value of $\bar{B}_c$ tends to 4.5 for all regular two-dimensional lattices[24,25] and to 2.7 for all three-dimensional lattices.[24] As we mentioned earlier, this limit must correspond to the zero-core randomly placed uniform circle and sphere problems we have solved. A glance at Tables II and III reveals that our answers are in good agreement with the regular lattice extrapolations.

We have determined the dependence of $\bar{B}_c$ on core size for site percolation on a random lattice. $\bar{B}_c$ is difficult to calculate from a knowledge of $R_c/2\bar{r}_s$ for these models, so we counted the number of bonds directly within our program. The results for two dimensions are given in Table II and in Fig. 12. Models with large core sizes

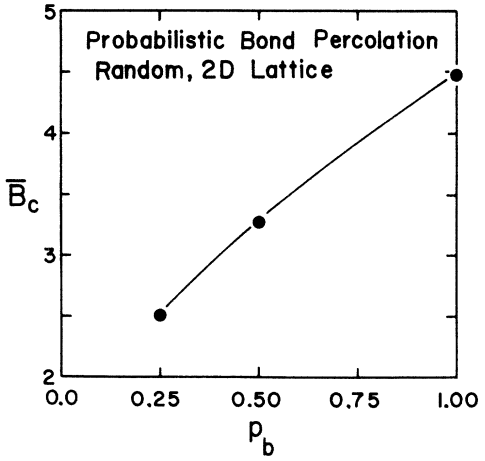

FIG. 13. Critical number of bonds per site for probabilistic bond percolation. For the random two-dimensional lattice, we show the dependence of $\bar{B}_c$ on the fraction p_b of possible bonds for a probabilistic bond model.

were difficult to study with our site placement algorithm, so no results for $r_{HC} > \bar{r}_s/\sqrt{2}$ were obtained. However, the general dependence is clearly demonstrated.

For the several zero-core models we have solved, only the site problems (uniform circles, squares, and spheres) seem to have an invariant value of $\bar{B}_c$. All the deterministic bond problems considered here have $\bar{B}_c$ lower than found for the site problem. For instance, the variable circles were found to percolate at $\bar{B}_c = 3.98$.

We originally thought that the probabilistic bond problem might possess an invariant $\bar{B}_c$, since it was this case on regular lattices which spawned the concept. However, Fig. 13 shows that as the probability for having a possible bond, p_b, drops from unity, the value of $\bar{B}_c$ also decreases markedly.

From a consideration of these results, we conclude that $\bar{B}_c$ is not a true dimensional invariant, but the concept may be useful as a secondary solution technique in some cases if proper consideration is given to its limitations.

VI. SUMMARY

We began this paper by formally defining the percolation problems. We emphasized particularly the role of the bonding function and the distinction between deterministic and probabilistic bonding parameters. Percolation models were divided into several categories which were useful in discussing problems on the random lattice but yet were compatible with previous definitions for the regular lattice.

Following a discussion of primary methods for obtaining percolative solutions, including our own, we presented the results of our Monte Carlo calculations for many random-lattice models. The models were chosen to illustrate the effect of hard-core interactions, probabilistic and deterministic bonding parameters, and various forms for the bonding function.

Using our random-lattice results and the regular lattice results of others, we have examined two secondary methods for solving percolation problems. Both the CVF concept and the $\bar{B}_c$ concept were found to be useful for this application in some cases. However, neither quantity was found to be a dimensional invariant as core-size effects and other factors affect their value significantly.

APPENDIX A: 2D CAF

In a recent paper, Zallen and Scher[10] posed a two-dimensional percolation problem for which they claimed an exact solution. Following their notation we let $\phi(E)$ be the area fraction available to carriers moving in a potential field as a function of their energy E. A particular value $E_{1/2}$ is defined by the relation, $\phi(E_{1/2}) = \frac{1}{2}$. They claim that if

$$\phi(E_{1/2} + \Delta E) + \phi(E_{1/2} - \Delta E) = 1, \qquad \text{(A1)}$$

then $\phi_c(E)$ = critical area fraction = $\frac{1}{2}$. By the following simple counterexample we wish to show that Eq. (A1) does not yield $\phi_c = \frac{1}{2}$.

Consider a model for which $\phi(E) = \frac{1}{2}$ for all E. Equation (A1) is clearly satisfied. An example of such a model is that of hard, nonoverlapping disks or circles of radius $r_{HC} = 1/\sqrt{2\pi N}$, where N is the two-dimensional density of sites. In the context of Zallen and Scher's paper this corresponds to carriers able to move within the disks but not through the intervening medium. Carriers are permitted to move from one disk to another only if the disks touch. If these disks are randomly distributed in space, we may then use the results of our hard-core calculations as presented in Fig. 7. From these results we can see that when $\phi = \frac{1}{2}$ $(r_{HC}/\bar{r}_s = 0.707)$ the bonding radius required for percolation, R_c, is larger than $2r_{HC}$. Thus the area fraction $\phi = (r_{HC}/\bar{r}_s)^2$ must be larger than $\frac{1}{2}$ for these disks to percolate when $R_c = 2r_{HC}$.

The above model is not the only example of when Eq. (A1) fails to guarantee $\phi_c = \frac{1}{2}$.[31] Furthermore the counterexamples are not limited to models with hard cores as zero-core instances are also found[31] with $\phi_c = 0.68$.

Using the terminology of Zallen and Scher, the symmetry expressed by Eq. (A1) is not sufficiently stringent to ensure that the critical area fraction for oceans and continents must be equal.

APPENDIX B: CVF FOR VARIABLE SPHERES

For the variable sphere and circle (deterministic bond) models considered in Sec. IV, OLF's may easily be constructed as shown in Fig. 5. Each site is assigned a random parameter E_i between zero and one. With the bonding condition that $d_{ij} \leq (E_i + E_j)r_m$, the radius associated with each site becomes $E_i r_m$, where r_m is the maximum radius. Let $N(E_i)dE_i$ be the density of sites with parameter value E_i to $E_i + dE_i$. Further let

$$A(E_i) = \pi E_i^2 r_m^2$$

and

$$V(E_i) = (4\pi/3)E_i^3 r_m^3.$$

These are the area and volume occupied by individual OLF's in the appropriate dimension. Since there is no hard-core exclusion in this problem, the probability that an arbitrary point (in the two-dimensional case) is *not* covered by a circle of radius $E_i r_m$ is[1] $\exp[-A(E_i)N(E_i)\,dE_i]$. The probability that an arbitrary point is not covered by any of the OLF's is then $\exp[-\int_0^1 A(E_i)N(E_i)\,dE_i]$.

Using the notation established in Sec. IV ($r_m = \frac{1}{2}R$)

and the uniform $N(E_i)$, one finds the critical area fraction to be

$$1 - \exp[-\tfrac{1}{3}(\pi R_c^2 N_s/4)] = 1 - \exp[-\tfrac{1}{3}(R_c/2\bar{r}_s)^2].$$

Likewise, the critical volume fraction in three dimensions is

$$1 - \exp[-\tfrac{1}{4}(4\pi R_c^3 N_s/24)] = 1 - \exp[-\tfrac{1}{4}(R_c/2\bar{r}_s)^3].$$

From Sec. IV we find numerically that the variable circles and spheres, respectively, percolate when the CAF is 0.680 and the CVF is 0.303.

APPENDIX C: $\bar{B}_c$ VERSUS DIMENSION

We wish to note here an interesting numerical relation observed between values of $\bar{B}_c$ for site percolation among zero-core randomly placed uniform "spheres" in d spatial dimensions. From our results $\bar{B}_c$ seems to obey the equation

$$(\bar{B}_c)^d = \text{const} \cong 20 \ . \qquad \text{(C1)}$$

For two dimensions Eq. (C1) yields $\bar{B}_c = 4.47$ compared to 4.48 found by us and 4.5 found by Dalton *et al.*[24] and by Domb and Dalton.[25] In three dimensions the equation gives $\bar{B}_c = 2.71$; we find 2.80 which, as we discuss in Sec. IV, should be slightly larger than the value of 2.7 from Domb and Dalton.[25] Equation (C1) is solved by $\bar{B}_c = 2.11$ in four dimensions, whereas we find 2.3 ± 0.2.

At this point Eq. (C1) is completely empirical. We present it in the hope that a study of this relation will lead to a quantitative understanding of the role of dimensionality within percolation theory.

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*Work supported by the U. S. Atomic Energy Commission.

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[20]Gilbert (Ref. 18) constructed random arrays of sites within a square in much the same way we do. However, for some unexplained reason his site density, N_s, varies with his chosen circle radius. For a given sample and a given radius he attempted to determine the fraction of sites that belong to the largest cluster, $P_{LC}(R, N_s)$. Postulating that this is approximately equal to the fraction of sites in an infinite cluster (for $N_s \to \infty$), i.e., $P_{LC}(R, N_s) = P_\infty(R, \infty)$, he estimates $R_c/2\bar{r}_s = 0.895$. Gilbert did say, and we concur, that his technique was not good for large cluster sizes, but he did not attempt a correction. Furthermore, we feel that the assumption concerning the equality, or near equality, of fractions is without justification.

[21]Roberts (Ref. 19) for two dimensions and Roberts and Storey (Ref. 27) for three dimensions generate a random array of sites. Using many samples, they determine the expected (or average) cluster size, $e(\bar{B})$, as a function of $\bar{B}$, the average number of bonds per site. ($\bar{B} \propto t$ of their notation.) By extrapolating $1/e(\bar{B})$ against $\bar{B}$, they claim to find the value $\bar{B}_c$ at which $e(\bar{B})$ first becomes infinite. We question this extrapolation procedure. For site percolation on regular lattices, Sykes and Essam (Ref. 11) have shown that near the critical point, $1/e(\bar{B}) \propto (\bar{B}_c - \bar{B})^{j+1}$, where $j = 11/8$ in 2D and $j = 11/16$ in 3D. This would imply that their extrapolation underestimates $\bar{B}_c$ and thus R_c. In 2D, their value of $R_c/2\bar{r}_s = 0.977 \pm 0.019$ is in fact lower than ours of 1.06. In 3D, Roberts and Storey get $R_c/2\bar{r}_s = 0.719 \pm 0.020$ where the uncertainty is three standard deviations. Our value of 0.704 is within their uncertainty, although we do not understand why their value is not lower.

[22]M. Pollak, J. Non-Cryst. Solids 11, 1 (1972).

[23]In Ref. 22 Pollak calculates a lower bound to the critical radius for the random site percolation model. His condition for the lower bound to the critical radius, $R_{c,lb}$, is $\sum_{n=1}^{\infty} p_n(R_{c,lb}) = 1$, where $p_n(R)$ is the probability that the nth nearest neighbor is at a distance R or less. This may be shown to imply that $R_{c,lb} = \bar{r}_s$ where $\bar{r}_s = 1/\sqrt{\pi N_s}$ in 2D and $(3/4\pi N_s)^{1/3}$ in 3D. In any dimension then, $R_c/2\bar{r}_s \geq 0.500$.

[24]N. W. Dalton, C. Domb, and M. F. Sykes, Proc. Phys. Soc. 83, 496 (1964).

[25]C. Domb and N. W. Dalton, Proc. Phys. Soc. 89, 859 (1966).

[26]The authors thank Dr. W. J. Camp for pointing this out

to them.
[27]F. D. K. Roberts and S. H. Storey, Biometrika 55, 258 (1968).
[28]D. F. Holcomb and J. J. Rehr, Jr., Phys. Rev. 183, 773 (1969).
[29]J. Kurkijarvi, Phys. Rev. B 9, 770 (1974).
[30]A. S. Skal and B. I. Shklovskii, Fiz.Tekh. Poluprovodn. 7, 1589 (1973). [Sov. Phys.-Semicond. 7, 1058 (1974)]. In addition to perolation among spheres, these authors solve problems with other 3D bonding criteria corresponding to cubes, tetrahedra, ellipsoids, double paraboloids, and several concave figures.
[31]G. Pike (unpublished calculations).