

Probabilistic Bond Percolation in Random Arrays

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We consider the problem of percolation in a system having sites distributed at random, but in which only a fraction h of the physical overlaps form viable links. We convert this to a site problem on the covering lattice, and then show that in two dimensions $h \simeq 1/S^4$ for $h \simeq 1$, and $h \simeq 4/S^2$ for $h \ll 1$, where S is proportional to the critical percolation radius in the original array. This result reproduces the $T^{-1/3}$ behavior for $\log(\text{conductivity})$ expected of variable-range hopping and found by numerical methods. It also accounts for the region of transition to r -percolation as $T \rightarrow \infty$. We make a prediction that in three dimensions, $h = 1/8S^3 + \text{const}/S^6$, but numerical confirmation is lacking for this case. While the argument is not exact, we have demonstrated a novel approach to random systems.

KEY WORDS: Percolation; random lattice; hopping conduction; two and three dimensions; $T^{-1/4}$ and $T^{-1/3}$ laws; scaling.

1. INTRODUCTION

The problem of percolation on regular lattices has been brought to an advanced state. However, in electrical conduction, interest centers on points that are randomly distributed in space, since such an array can be used to represent an amorphous substance conducting through a hopping mechanism. A number of approaches have been adopted to calculate critical limits for percolation in such arrays. These include modeling by means of Cayley trees,⁽¹⁾ analyses of the statistics of chain length,^(2,3) Monte Carlo studies of site overlap,⁽⁴⁾ and extension to random arrays of a number of empirical rules that are found to hold on regular lattices.

The Cayley tree approach provides valuable guidance because it provides a soluble model, albeit a somewhat unphysical one. The results may be closer to the behavior on real lattices than one might expect from the

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model, partly because clusters become treelike near the percolation limit⁽⁶⁾ (although this has been disputed⁽⁶⁾) and partly because the fraction of cyclic closures is only a few percent of the total number of bonds.⁽⁷⁾ Nevertheless, it must be said that the Cayley tree is unlikely to provide accurate percolation limits for two- and three-dimensional systems. The chain statistics method gives numerical results that are very sensitive to the details of the criterion adopted to describe percolation,⁽⁸⁾ so is also an unreliable guide.

Empirical rules have been found to hold in a number of cases (see e.g. the review by Shante and Kirkpatrick⁽⁹⁾). The critical volume fraction (CVF) is useful for the *site problem* on regular lattices, but is not applicable to random systems,⁽⁴⁾ apart from restricted cases.⁽¹⁰⁾ The mean bond number at percolation \bar{B}_c for the site problem approaches the limits of 4.5 ($d = 2$) and 2.8 ($d = 3$) as the bonding range increases above the lattice constant. Here, d is the number of dimensions. These invariants also hold for random arrays of spherical sites, but only if the sites are uniform in size. The *bond problem* on regular lattices yields \bar{B}_c as an approximate invariant with the value $d/(d - 1)$, and irregular lattices obtained by topological distortion of regular lattices^(11,12) naturally give the same result. However, the bond problem on truly random arrays is not definable in any direct way, and \bar{B}_c is certainly not constant for the case discussed in this paper. The Cayley tree result is $\bar{B}_c = z/(z - 1)$, where z is the coordination number, and comparable formulas apply for various cactii.^(13,14) This expression corresponds to the most efficient interconnection between sites, because of the lack of closed loops, so it provides an absolute minimum value for all arrays. It contains no dimensional dependence, and in general it is a mediocre approximation to the correct results.

We are finally brought to the Monte Carlo computation of the site problem as being the one method of attack in which a well-defined problem can be posed, a well-defined answer can be obtained, and the model bears some reasonable resemblance to amorphous materials. In practice, however, we do not expect every physical overlap of sites to lead to a conductive link. The AHL interaction,⁽¹⁵⁾ or some similar formulation, places energy restrictions as well as spatial restrictions upon the formation of links. This has been incorporated in the Monte Carlo approach by dealing with overlap in a $(d + 1)$ -dimensional space having energy as the additional coordinate.⁽¹⁶⁾ Unfortunately, the problem becomes rather less manageable numerically, and these authors were forced to make comparisons by using their exact results for spherical sites⁽⁴⁾ and applying them to the nonspherical sites in $(d + 1)$ dimensions. This procedure is known to give misleading answers (Table 3 of Ref. 10).

An alternative and somewhat simpler approach is to ignore the explicit energy dependence, but to assume that some fraction $1 - h$ of the links

that would result from spatial overlap considerations alone are rendered inoperative because they are inhibited by the energetics or for other reasons, such as misalignment of wave functions. When this fraction of the links is chosen at random we have the *probabilistic bond* model, also evaluated by Seager and Pike. These authors found that as the retained fraction h was reduced, and the critical radius correspondingly increased to hold the system at the percolation limit, the mean bond number \bar{B}_c fell. This was contrary to expectation, because the procedure of increasing the critical radius to a value much greater than the average site spacing is similar to the situation on regular lattices in which bonding between second nearest neighbors, third nearest neighbors, etc., leads to the invariant \bar{B}_c mentioned above. The essential difference between the two procedures seems to lie in the fact that the sites are thinned out in the regular lattice case, while the bonds are thinned out here.

Since this probabilistic bond model can be interpreted rather directly in terms of an energy restriction, it is desirable to understand why \bar{B}_c varies with h in the way it does, and we offer a partial explanation, which accounts for the published numerical results for $d = 2$. The more interesting case of $d = 3$ does not seem to have been done numerically, because of the sheer size of the computational work, but we suggest what the result might be.

2. THEORY

2.1. The Site Problem in the Covering Lattice

We consider a random array of circular sites on a plane. There are N_s circles per unit area, their radius is R (this is the inclusive figure or IF radius), and any amount of overlap is permitted (no hard core). A mean spacing r_s is defined by

$$\pi N_s r_s^2 = 1 \tag{1}$$

A link is formed whenever one circle overlaps the center of another, and a link corresponds to a bond being attached to each site. The number of bonds on a site is B , which is a Poisson variate with mean value \bar{B} given by

$$\bar{B} = \pi R^2 N_s = 4(R/2r_s)^2 \tag{2}$$

If R is steadily increased from zero, then eventually infinitely long connected paths occur at a critical radius R_c . The corresponding critical bond number is \bar{B}_c . Now the radius is further increased, so that \bar{B} exceeds this number, and the system is well beyond the percolation limit. Then a fraction $1 - h$ of the bonds are removed by a random selection procedure,

Table I. Parameters of the Thinned Lattice Calculations^a

h	S	\bar{B}_c	\bar{B}_{cc}	h_{calc}
1.0	1.058 ± 0.026	4.48	7.06	0.998
0.5	1.28	3.28	4.81	0.514
0.25	1.585	2.51	3.46	0.253

^a h is the fraction of bonds retained after increase of bonding radius; S is the reduced OLF radius $S = R_c(h)/2r_s$ (data from Pike and Seager⁽⁴⁾); \bar{B}_c is the mean bond number (data from Pike and Seager⁽⁴⁾); \bar{B}_{cc} is the mean bond number in the covering lattice [Eq. (5)]; h_{calc} is the fraction calculated using Eq. (17) and the given values of S .

until the system is reduced once more to the point of percolation. It is found that the now augmented $R_c(h)$ is accompanied by a reduced $\bar{B}_c(h)$. The available numerical results of Pike and Seager⁽⁴⁾ are reproduced in Table I for reference.

It is not possible to construct a theory ab initio to account for the more effective interconnection in the new array from which bonds have been thinned, and we proceed by a scaling argument. We recall that a bond problem on a direct lattice can be converted into a site problem on the corresponding covering lattice.⁽¹⁷⁾ The sites of the covering lattice are located at the centers of the links of the direct lattice, and links in the covering lattice are made between all sites for which the corresponding bonds in the direct lattice have a common vertex. It is clear from Fig. 1 that a link in the direct lattice that connects two sites having i and j bonds on them corresponds to a site in the covering lattice that has $i + j - 2$ bonds.

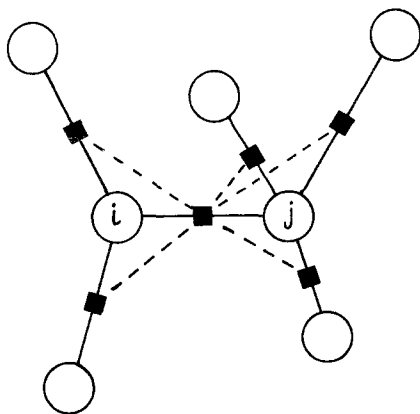


Fig. 1. Construction of the covering lattice. The direct lattice sites are circles, the covering lattice sites are squares. The labeled direct sites have $i = 3$ and $j = 4$ bonds, so the covering lattice site between them has $3 + 4 - 2 = 5$ bonds.

The onset of bond percolation in the direct lattice is accompanied by the onset of site percolation in the covering lattice, and the latter is more easily handled because all sites contribute in the normal way to percolation in this array: The fraction $1 - h$ of links that have been suppressed in the direct lattice do not enter into the transformation. Now we make the hypothesis that the sites in the covering lattice are randomly placed, circular, uncorrelated, and all have the same effective radius. Then the covering lattice will percolate when its mean bond number \bar{B}_{Cc} equals $\bar{B}_c(1)$. We use the subscript C to denote quantities in the covering lattice. In the thinned direct lattice, the mean bond number is

$$\bar{B}_c(x) = 4hS^2 \quad (3a)$$

where

$$R_c(h)/2r_s = S \quad (3b)$$

If we substitute this value for both i and j , we obtain

$$hS^2 = [\bar{B}_c(1) + 2]/8 = 0.81$$

This suggests that hS^2 is a constant. It is obvious from the data that this does not hold in the range $1 \leq h \leq 0.25$. We can trace the failure of this procedure to at least two defects in the hypothesis. The distribution of the bonds on the sites of the covering lattice is not in fact of Poisson form. If the fraction of sites in the direct lattice having i bonds is written q_i , then the probability of finding a link that joins sites having i and j bonds is proportional to the term in $q_i q_j$ contained in the pair probability

$$(q_0 + q_1 + \dots + q_n + \dots)^2 \quad (4)$$

where

$$q_n = \frac{\bar{B}^n}{n!} \exp(-\bar{B})$$

The resulting probabilities q_{Cn} that sites have n bonds in the covering lattice are readily calculated, and deviate markedly from the Poisson distribution. The corresponding mean bond numbers \bar{B}_{Cc} have also been calculated, using

$$\bar{B}_{Cc} = \sum nq_{Cn} \quad (5)$$

and these are displayed in Table I. They are by no means constant.

The second defect in our original set of hypotheses is that there will in fact be correlation between sites in the covering lattice, because a direct lattice site having i bonds, where i is large, gives rise to a group of i interlinked sites in the covering lattice, having at least $i - 1$ bonds each. Whether

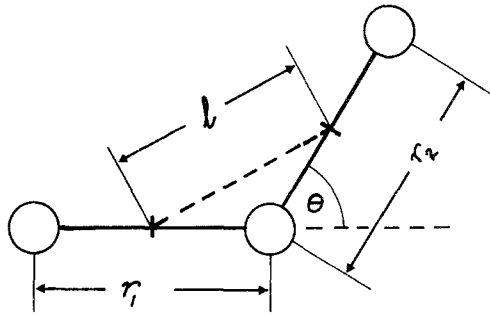


Fig. 2. Bond length l in the covering lattice related to the parameters r_1 , r_2 , and θ in the direct lattice.

this correlation leads to a preferential directivity of bonds, i.e., effectively noncircular sites, is a problem we have not investigated. Nor have we assessed whether the covering lattice sites will have spatial correlations in addition to bond number correlations.

We now turn to a calculation of the length distribution of links in the covering lattice. The length can be easily evaluated from the cosine formula, as shown in Fig. 2:

$$(2l)^2 = r_1^2 + r_2^2 + 2r_1r_2 \cos \theta$$

where l is the new link length, r_1 and r_2 are the link lengths in the direct lattice, and θ is the polar angle. These quantities are distributed randomly with probability distributions

$$p(r_1^2) d(r_1^2) = d(r_1^2)/R_c^2, \quad r_1 < R_c$$

$$p(r_2^2) d(r_2^2) = d(r_2^2)/R_c^2, \quad r_2 < R_c$$

$$p(\theta) d\theta = d\theta/2\pi \quad (d = 2)$$

$$= \frac{1}{2} \sin \theta d\theta \quad (d = 3)$$

The maximum link length in the covering lattice is of course the critical radius in this system, so we have

$$R_c = R_{c_c} \quad (6)$$

The two-dimensional calculation leads to a cumbersome quadrature, so the integral distribution $P(\lambda^2)$ has been evaluated by direct numerical integration of the probability distributions. Here, $\lambda = 2l/R_c$. We have confirmed our numerical procedure by evaluating the three-dimensional case in the same way, and checking it against the simple analytic result for $3d$. Details of the analysis are given in Appendix A, and the results are plotted in Fig. 3.

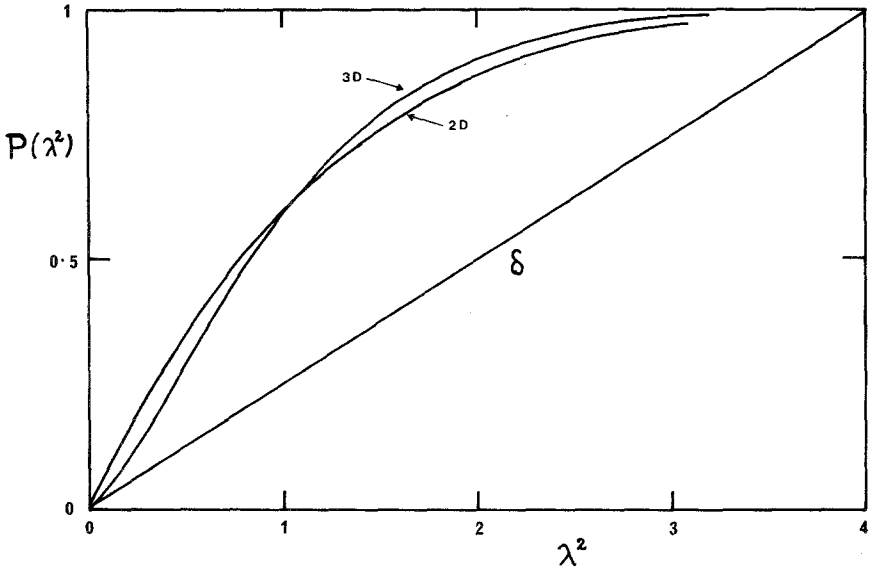


Fig. 3. Integral distribution of λ^2 as a function of λ^2 , where λ is the reduced bond length. The curves are for a covering lattice of a random direct lattice in two and three dimensions, while the straight line (δ) gives the distribution corresponding to a set of circles or spheres all having the same radius.

It is clear that the same relative distribution holds, whatever the value of R_c . The natural assumption to make is that this corresponds to the unique site radius in the covering lattice that is scaled relative to R_c , and is given by Eq. (6). However, we show in Fig. 3 that the bond length distribution corresponding to sites of uniform radius differs considerably from the distributions we have derived. It follows that if the conversion to a site problem on the covering lattice is in any sense meaningful, then we must be dealing with sites of varying size. The concept of the inclusive figure is now inapplicable, and we have to work with the overlapping figure (OLF) radii X_c , having a maximum value

$$X_{cc} = \frac{1}{2}R_c \tag{7}$$

This conclusion automatically leads to a bond distribution of non-Poisson form. Whether this failure of the Poisson distribution is consistent with the failure associated with Eq. (4) remains to be established. A distribution of the radii X_c that is scaled relative to R_c would give rise to a constant value of the mean bond number \bar{B}_{cc} , and in principle it can be calculated from the probability density $p(\lambda^2)$. The computation is not straightforward, and it is discussed in Appendix B.

2.2. Scaling and the Constant-Volume-Fraction Result

The regularity of the link length distribution $p(\lambda^2) d\lambda^2$ in the covering lattice suggests strongly that there should be some scaling relations between the relevant quantities in the covering lattice. The site density in the covering lattice is the same as the link density $\rho(h)$ in the direct lattice:

$$N_{Cs} \equiv \rho(h) = 2hN_s S^2 \quad (8)$$

and this can be used to define the mean site radius r_{Cs} in the covering lattice:

$$\pi N_{Cs} r_{Cs}^2 = 1 \quad (9)$$

If the sites in the covering lattice were uncorrelated, then a straightforward extension of an earlier calculation⁽¹⁰⁾ shows that at percolation one would have

$$\bar{B}_{Cc} = k(X_{Cc}/r_{Cs})^2 \quad (10)$$

in which X_{Cc} is the overlapping figure (OLF) critical radius, and k is a number that can be calculated if the distribution of OLF radii is known. Since $X_{Cc} = \frac{1}{2}R_c$, we would obtain by substitution

$$\bar{B}_{Cc} = 2khS^4 \quad (\text{no correlation}) \quad (11)$$

This would suggest that hS^4 is a constant. However, we already know from the earlier discussion that there is correlation, so that k may not be a constant, and we also know that \bar{B}_{Cc} varies. In fact, hS^4 is not a constant for the values given in Table I. It shows a 19% variation, while the uncertainty in S^4 is about 14%.

However, we can obtain the same scaling result in a way that does not require the hypothesis that bonding be uncorrelated. We merely have to postulate that percolation occurs in the covering lattice when the mean site separation falls below some fixed fraction f of the maximum separation at percolation. Thus

$$r_{Cc} \leq 2fX_{Cc} \quad (12)$$

and on substituting the previous results (3b) and (7)–(9), we get

$$1 \leq 8f^2 hS^4 \quad (13)$$

If the sites can be regarded as circular but with variable radii, then their mean area at percolation \bar{V}_{Cc} is some weighted fraction ω of the maximum area. Thus

$$\bar{V}_{Cc} = \pi X_{Cc}^2 \omega \quad (14)$$

The critical area fraction (CVF) is given by

$$\exp(-N_{Cs} \bar{V}_{Cc}) = 1 - \text{CVF} \quad (15)$$

The CVF seems to be an invariant for overlapping disks with size distributions,⁽¹⁰⁾ and therefore $N_{Cs}\bar{V}_{Cc}$ should also be invariant. Hence we expect

$$-\ln(1 - \text{CVF}) = \pi\omega N_{Cs}X_{Cc}^2 = \omega(X_{Cc}/r_{Cs})^2 \tag{16}$$

and this is the same as Eq. (13), with $\omega/4f^2 \equiv -\ln(1 - \text{CVF})$. Pursuing this argument, we know that $\text{CVF} \simeq 0.68$ in two dimensions, and thus it follows from the values $h = 1$ and $S = 1.058$ given in Table I that $\omega = 0.45$.

We have in Eq. (13) a strong suggestion that hS^4 should be constant. However, this should not hold at very small h , because when the bond density is dilute, the bonding becomes very efficient. The most efficient process known is percolation on Cayley trees, where $\bar{B}_c = z/(z - 1)$, and z is the coordination number of the site. We expect the thinned direct lattice to approach the value $\bar{B}_c = 1$ ($z = \infty$) because (1) finite clusters grow treelike (ramified) as they approach the percolation threshold from below^(5,18) on regular lattices, (2) the connected paths just above percolation on regular lattices show only a few percent of bonds devoted to cyclic closures,⁽¹⁹⁾ (3) at least one system modeling random sites shows the same lack of cyclic bonds,⁽⁷⁾ and (4) the random system under study in this paper does have $z = \infty$. Hence hS^4 does not extrapolate to the correct limit. In fact, to be consistent with the tree limit, we expect

$$\lim_{h \rightarrow 0} 4hS^2 = 1$$

which has the same form as Eq. (3). Hence we put forward the combination

$$h = \frac{1}{4S^2} + \frac{0.97}{S^4} \tag{17}$$

The coefficient of S^{-4} is found by fitting this equation at $x = 1$, and it has the values 1.01 and 0.97 obtained from assemblages of 1000 and 4000 points, respectively. In Table I we give the fit to Eq. (17), and we see that it differs from the known h for 4000-point samples by about 3%, well inside the uncertainty in S^4 . If this approach is correct, then comparison of Eq. (7) and (13) yields the value $8f^2 = (0.97)^{-1}$, and substitution into Eq. (16) gives $\omega = 0.58$, ignoring the term $1/4S^2$. The value of ω becomes smaller, and no longer a true constant, if this term is included.

We can now see that equivalent arguments for a three-dimensional problem would lead to an equation of the form

$$h = \frac{1}{8S^3} + \frac{c}{S^6} \tag{18}$$

where again the term in S^{-3} represents the dilute limit. The value $S = 0.7048$ at $h = 1$ gives a value for the constant of $c = 0.0788$, while it comes to 0.122

if the first term is omitted. Since the first term is already 36% of the total at $h = 1$, it ought to be quite straightforward to establish by numerical methods whether it does in fact have to be taken into consideration, whereas we have seen that the two-dimensional data are not decisive.

3. DISCUSSION

We have suggested that it is possible to understand the behavior of the percolation threshold in random two-dimensional arrays in which some random bond deletion occurs in terms of a scaling type of behavior, in which the leading result is $hS^4 \simeq \text{const}$. While the available data match this result, with minor adjustments, we are obliged to point out that there are a number of reasons why this approach needs to be treated cautiously at present. The first is that the numerical data⁽⁴⁾ on percolation limits were obtained by arbitrarily picking the median value of the critical radius R_c for a relatively small set of trials at each value of x . There is thus some conceptual uncertainty as to whether the median is indeed the proper value to use, as well as the more trivial uncertainty associated with its rather wide confidence limits.

The second objection is a more technical one. The relation between the bond length distribution $p(\lambda^2)$ and the presumed normalized distribution of radii $g(E)$ is developed in Appendix B. It is shown there that the value of ω is 0.32. Thus it is somewhat smaller than the values predicted by the scaling assumptions made here. However, we have not been able to construct a $g(E)$ that generates our known $p(\lambda^2)$. While the discrepancy seems to be of a qualitative nature, it may be merely a question of quantitative adjustment of trial distributions.

The final problem is the matter of correlation. By going to the covering lattice, we have converted the thinned bond problem to what ought to be the simpler site problem, rather than choosing the renormalization group method.⁽²⁰⁾ We have not, however, made any allowance for the existence of close groups of sites, all having large bond numbers, which probably occur in the covering lattice. It may well be that this leads to relatively strong perturbation of our simple theory, and so may account for the discrepancies mentioned in the previous paragraph.

It is pertinent to ask how the present calculation matches the variable-range hopping formulation of amorphous conduction.⁽²¹⁾ If the jump probability between two sites is proportional to $\exp(-\xi)$, where

$$\xi = 2\alpha r + \Delta E/kT \quad (19)$$

where α is a measure of the rate of decay of the site wave functions and ΔE is a measure of the energy difference, then the percolation approach

asserts that for critical percolation, there is some maximum value ξ_c , and all less probable jumps can be ignored. This assumption leads directly to the same temperature dependence as found for variable-range hopping^(15,16,22) for the temperature range over which the energy term is important (z -percolation region). We note that at a range r , the fraction y of physically overlapping bonds that may tunnel is given by

$$y \simeq (kT/W)(\xi_c - 2\alpha r)$$

where W is the half-width of the impurity distribution, which is assumed to have a more or less constant density of states near the Fermi level. We show in Appendix C that this has a mean value \bar{y} given by

$$\begin{aligned} \bar{y} &= kT\xi_c/3W, & kT\xi_c/W < 1 \\ &= 1 - (W/kT\xi_c) + (W/kT\xi_c)^2/3, & kT_c/W > 1 \end{aligned} \tag{20}$$

In the present calculation, we are simulating the effect of the energy term by saying that only a fraction h of the bonds due to physical overlap actually contributes to the conduction process. If we ignore the detailed change of y with radius, and boldly equate \bar{y} with h , then we have a connection between S , given by Eq. (17), and the temperature from Eq. (20). Since the conductivity σ is given by

$$\sigma \propto \exp(-\xi_c) \propto \exp(-2\alpha r_s S) \tag{21}$$

this amounts to an implicit relation between conductivity and temperature. In the low-temperature limit (S large) we have the approximate relation

$$2\alpha r_s S k T \xi_c / 3W \simeq 1/4S^2 \tag{22}$$

which immediately yields the relation $\sigma \propto \exp(-\text{const} \times T^{-1/3})$, exactly as found by the variable-range hopping technique. It is in this temperature range that the replacement of \bar{y} by h will be most satisfactory, because here the formation of conducting links is strongly forbidden on energetic grounds, with the radius effect playing a minor additional role. The complete temperature dependence is plotted in Fig. 4. The corresponding three-dimensional calculation using Eq. (18) leads to the familiar $T^{-1/4}$ law for the temperature dependence of conductivity. Clearly the form of our "correction" term in Eq. (17) is all important.

We have shown that by means of scaling arguments it is possible to account for the numerical results of Pike and Seager⁽⁴⁾ on the percolation limit when some bonds chosen at random are rendered ineffective. These arguments apply at relatively small suppressions ($h \gtrsim 0.25$), and are overtaken in the low-temperature limit (strong inhibition) by the Cayley-tree result, which in fact coincides with the criterion of constant link density discussed earlier. We have noted that the scaling argument is not exact.

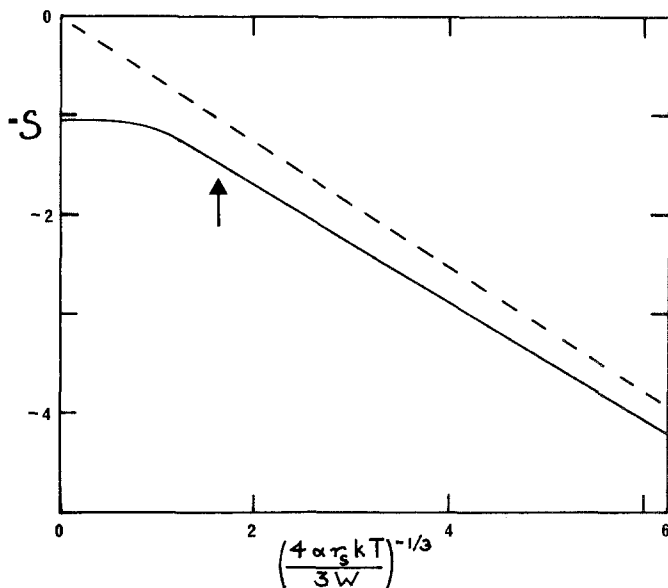


Fig. 4. Logarithmic plot of conductivity σ against $T^{-1/3}$ for a two-dimensional random lattice, where $\ln \sigma = -2\alpha r_s S$. The arrow marks the change from intermediate behavior to the variable-range hopping regime ($kT\xi_c/W = 1$). The dashed curve gives the asymptotic limit of Eq. (22). At the left we go from the intermediate region to r -percolation as $T \rightarrow \infty$.

Despite these difficulties, we think that we have investigated a possible alternative route, which may lead to further understanding of the problem of percolation on random lattices, and we have made quantitative predictions for the three-dimensional problem, which now need to be tested by numerical methods.

APPENDIX A. CALCULATION OF THE BOND LENGTH DISTRIBUTIONS IN THE COVERING LATTICE

The calculation of the distribution of bond lengths described by Fig. 2 is most readily carried out by using reduced variables $x = r_1/R_c$, $y = r_2/R_c$, and $z = \cos \theta$. We give an outline of the calculation for the three-dimensional case, which leads to a simple analytic result. We start from the normalized distribution functions for x , y , and z :

$$\begin{aligned}
 f(x) dx &= 2x dx, & g(y) dy &= 2y dy \\
 p(\theta) d\theta &= \frac{1}{2} \sin \theta d\theta, & h(z) dz &= p(\theta) |d\theta/dz| dz = \frac{1}{2} dz
 \end{aligned}$$

The normalized link length λ ($0 < \lambda < 2$) is given by

$$\lambda^2 = x^2 + y^2 + 2xyz$$

and standard methods give the distribution function of this variable as

$$p(\lambda^2) = \iiint dx dy dz f(x)g(y)h(z) \delta[q(z)]$$

where

$$q(z) = \lambda^2 - x^2 - y^2 - 2xyz$$

Now if z_0 is the value of z that makes $q(z) = 0$, then we can perform the integration over z to find

$$\begin{aligned} p(\lambda^2) &= \iint dx dy f(x)g(y)h(z_0)/|q'(z_0)| \\ &\equiv \iint dx dy \end{aligned}$$

The region of integration is given by

$$-1 \leq z \leq 1, \quad \lambda^2 = x^2 \pm 2xy + y^2$$

and corresponds to the shaded region in Fig. 5. The area is easily evaluated and gives directly

$$\begin{aligned} p(\lambda^2) &= 2\lambda - 3\lambda^2/2 \quad (0 < \lambda < 1) \\ &= (2 - \lambda)^2/2 \quad (1 < \lambda < 2) \end{aligned}$$

and the integral distribution is

$$\begin{aligned} P(\lambda^2) &= 4\lambda^3/3 - 3\lambda^4/4 \quad (0 < \lambda < 1) \\ &= -1/3 + 2\lambda^2 - 4\lambda^3/3 + \lambda^4/4 \quad (1 < \lambda < 2) \end{aligned}$$

This distribution is plotted in Fig. 3.

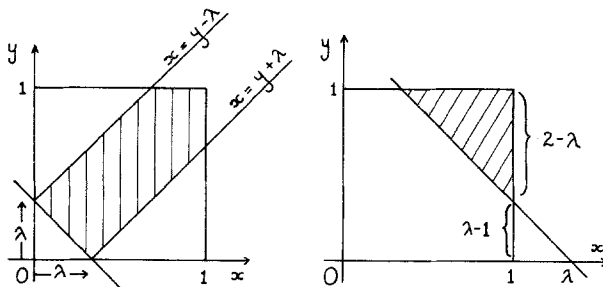


Fig. 5. Regions of integration for evaluating the integrals in Appendix A. The diagrams correspond to $\lambda < 1$ and $\lambda > 1$.

The corresponding calculation in two dimensions leads to

$$p(\lambda^2) = \frac{4}{\pi} \iint \frac{dx dy xy}{[4x^2y^2 - (x^2 + y^2 - \lambda^2)^2]^{1/2}}$$

with the same region of integration. The substitutions

$$\xi = (x + y)/\lambda, \quad \eta = (y - x)/\lambda$$

enable us to integrate over one variable, leading to

$$p(\lambda^2) = \frac{\lambda^2}{\pi} \int_0^1 d\eta \left(\frac{1}{2(1 - \eta^2)^{1/2}} \{ \zeta(\zeta^2 - 1)^{1/2} - \ln[\zeta + (\zeta^2 - 1)^{1/2}] \} \right. \\ \left. + (1 - \eta^2)^{1/2} \ln[\zeta + (\zeta^2 - 1)^{1/2}] \right) \\ \zeta = 2/\lambda - \eta, \quad 0 \leq \lambda \leq 1$$

and also

$$p(\lambda^2) = \frac{\lambda^2}{\pi} \int_1^{2/\lambda} d\xi \left\{ \frac{1}{2(\xi^2 - 1)^{1/2}} [\beta(1 - \beta^2)^{1/2} + \sin^{-1} \beta] \right. \\ \left. + (\xi^2 - 1)^{1/2} \sin^{-1} \beta \right\} \\ \beta = 2/\lambda - \xi, \quad 1 \leq \lambda \leq 2$$

We have not found a method of evaluating these integrals directly, though it is straightforward to obtain the limiting values

$$\lim_{\lambda \rightarrow 0} p(\lambda^2) = 1 - 2\lambda/\pi$$

$$\lim_{\lambda \rightarrow 2} p(\lambda^2) = 2\sqrt{2} \lambda^{1/2} (2 - \lambda)^{3/2} / 3\pi \simeq 4(2 - \lambda)^{3/2} / 3\pi$$

We have evaluated $p(\lambda^2)$ by a numerical method, directly from the probability distribution functions $f(x)$, $g(y)$, and $p(\theta)$. The three-dimensional result agrees with the analytic solution, and so we are confident that the two-dimensional result shown in Fig. 3 is also correct.

APPENDIX B. RELATION BETWEEN BOND LENGTH DISTRIBUTION, SITE RADIUS DIRECTION, AND MEAN AREA IN TWO DIMENSIONS

In the body of the paper, we have considered the distribution of bond lengths $p(\lambda^2)$ in the covering lattice derived from a direct lattice that has a positionally random distribution of sites in either two or three dimensions. Our arguments are then based on the assumption that the site problem in

the covering lattice can be treated, at least to a first approximation, as if each site could be assigned an effective radius EX_{Cc} , where X_{Cc} is the maximum physical radius of the site. The quantity EX_{Cc} is the radius of the overlapping figure (OLF).^(4,10) The parameter E is a random variable, $0 \leq E \leq 1$, and it has a normalized probability distribution function $g(E)$. It does not seem to be easy to derive $g(E)$ from $p(\lambda^2)$, but the converse is relatively simple using an extension of an earlier method.⁽¹⁰⁾ The number of links that have lengths lying in an interval $X_{Cc} dE$ is

$$dm = (X_{Cc}/r_{Cs})^2 d\lambda^2 \left[1 - \int_0^\lambda dE_0 g(E_0) \int_0^{\lambda-E_0} dE_1 g(E_1) \right], \quad 0 < \lambda < 1 \quad (\text{B1})$$

$$dm = (X_{Cc}/r_{Cs})^2 d\lambda^2 \int_{\lambda-1}^1 dE_0 g(E_0) \int_{\lambda-E_0}^1 dE_1 g(E_1), \quad 1 < \lambda < 2 \quad (\text{B2})$$

The right-hand sides of this pair of equations are the unnormalized forms of $p(\lambda^2)$. At first sight, it seems attractive to attack these equations by a Laplace transform method, because if we write

$$k(\lambda) = dm/d\lambda^2$$

then we obtain

$$dk/d\lambda = -(X_{Cc}/r_{Cs})^2 \int_0^\lambda g(x)g(\lambda-x) dx, \quad 0 < \lambda < 1 \quad (\text{B3})$$

$$dk/d\lambda = -(X_{Cc}/r_{Cs})^2 \int_{\lambda-1}^1 g(x)g(\lambda-x) dx, \quad 1 < \lambda < 2 \quad (\text{B4})$$

In fact, the definition that $g(E) = 0$ outside the range $0 < E < 1$ permits us to write these equations in the form of a convolution (B3) for all values of λ .

We use the abbreviation $(X_{Cc}/r_{Cs}) = S_C$, and then find that

$$s\mathcal{K}(s) - k(0+) = -S_C^2 \mathcal{G}^2(s) \quad (\text{B5})$$

and

$$\mathcal{K}(s) + s\mathcal{K}'(s) = -2S_C^2 \mathcal{G}(s)\mathcal{G}'(s) \quad (\text{B6})$$

$$2\mathcal{K}'(s) + s\mathcal{K}''(s) = -2S_C^2 [\mathcal{G}'^2(s) + \mathcal{G}(s)\mathcal{G}''(s)] \quad (\text{B7})$$

where $\mathcal{K}(s)$ and $\mathcal{G}(s)$ are the Laplace transforms, and the prime indicates differentiation with respect to the transform variable s . Using the fact that $k(\lambda)$ is finite and $k'(\lambda) = 0$ as $\lambda \rightarrow \infty$, we obtain the following limits:

$$\begin{aligned} k(0+) &= S_C^2 \mathcal{G}^2(0), & \mathcal{K}(0) &= -2S_C^2 \mathcal{G}(0)\mathcal{G}'(0) \\ \mathcal{K}'(0) &= -S_C^2 [\mathcal{G}'^2(0) + \mathcal{G}(0)\mathcal{G}''(0)] \end{aligned} \quad (\text{B8})$$

Using the general property that for a normalized distribution function such as $g(E)$ that $\mathcal{G}(0) = 1$ and $\langle E^n \rangle_g = (-1)^n (d^n \mathcal{G} / ds^n)_{s=0}$, we can write Eqs. (B8) in the form

$$\begin{aligned} k(0+) &= S_C^2, & \mathcal{K}(0) &= 2S_C^2 \langle E \rangle_g \\ -\mathcal{K}'(0) &= S_C^2 (\langle E \rangle_g^2 + \langle E^2 \rangle_g) \end{aligned} \quad (\text{B9})$$

Now the weighted area fraction ω used in the text is given by

$$\omega = \langle E^2 \rangle_g = -\mathcal{K}'(0)/S_C^2 - [\mathcal{K}(0)/2S_C^2]^2 \quad (\text{B10})$$

It also follows that

$$-s\mathcal{K}(s)/S_C^2 + 1 = \mathcal{G}^2(s) \quad (\text{B11})$$

In principle, we could put in trial solutions for $g(E)$ and use Eq. (B11) to derive $k(\lambda)$, which could then be compared directly with the computed bond distribution discussed in Appendix A. However, the finite range of E forces the Laplace transforms to be quite complicated and makes the inversion of $\mathcal{K}(s)$ impracticable.

The next method of attack is to use the convolution integral (B3) directly, performing the integration directly. Since it follows from the results of Appendix A that $g(E)$ becomes infinite at both ends of its range, some care is required to remove these singularities before numerical evaluation. We show in Fig. 6 the results of using the form

$$g(E) = A/E^{1/2}; \quad k(\lambda)/S_C^2 = (1 - \pi A^2 \lambda), \quad \lambda < 1; \quad A = 1/2; \quad \omega = 0.2$$

which clearly underestimates the fraction of circles having large radii and so underestimates ω . It does give a linear dependence of $k(\lambda)$ upon λ for $\lambda < 1$, though the slope is wrong. This particular form can be handled wholly analytically.

We also show the result obtained using

$$\begin{aligned} g(E) &= A/E^{1/2} + B/(1 - E)^{1/4} + C, & k(\lambda)/S_C^2 &= (1 - \pi A^2 \lambda), \quad \lambda \ll 1 \\ A &= \sqrt{2}/\pi, & B &= 1/[\pi^{1/4} \Gamma(\frac{3}{4})] = 0.613, & C &= -0.718 \\ 2A + (4/3)B + C &= 1, & \omega &= 0.281 \end{aligned}$$

Here, the value of A has been chosen to force the correct slope at $\lambda = 0$, and the value of B to obtain the correct limiting form at $\lambda = 2$, and C follows from the normalization of $g(E)$. This is a much better fit, but still underestimates the proportion of circles having large radii. It is obviously possible to make more elaborate choices for $g(E)$ to improve the fit, but this seems to be an exercise of limited value.

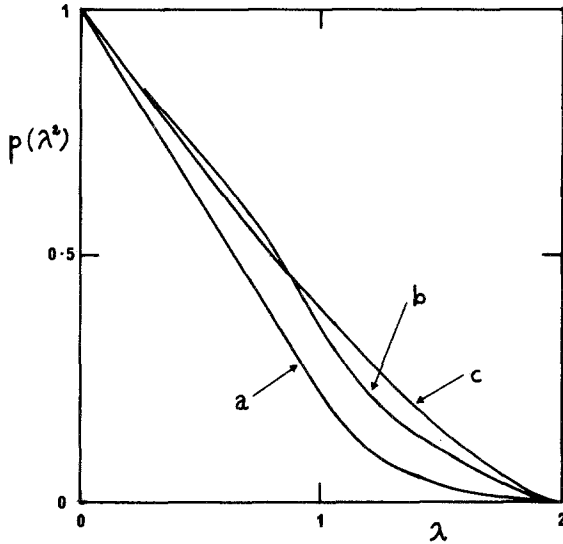


Fig. 6. Two-dimensional case. Plot of the distribution function $p(\lambda^2)$ as a function of λ in the covering lattice. Case (a), derived from $g(E) = A/E^{1/2}$. Case (b), derived from $g(E) = A/E^{1/2} + B/(1 - E)^{1/4} + C$. Case (c), given by numerical integration as outlined in Appendix A. In two dimensions only, $p(\lambda^2) = (dm/d\lambda^2)/S_c^2$.

We estimate ω directly by the following stratagem. The integral distribution $P(\lambda^2)$ is given to within about ± 0.02 by

$$\begin{aligned}
 P(\lambda^2) &\simeq \lambda^2 - 4\lambda^3/3\pi && 0 < \lambda < 1 \\
 &\simeq 1 - (32/15\pi)(2 - \lambda)^{5/2}[1 - 5(2 - \lambda)/14], && \lambda < 1 < 2
 \end{aligned}$$

and $dP/d\lambda^2 = 1$ at $\lambda = 0$. Now, by definition,

$$\bar{B}_{Cc} = \int_{\lambda=0}^2 dm \equiv M(X_{Cc}/r_{Cs})^2$$

where the multiplier M is formally found by integration of the λ -dependent parts of the right-hand sides of (B1) and (B2) over their respective ranges, and summing. This quantity lies in the range $0 < M \leq 4$, with the upper limit corresponding to the case of uniform circles [$g(E) \equiv \delta(1 - E)$]. The normalized bond distribution is thus $(dm/d\lambda^2)/MS_c^2 \equiv dP/d\lambda^2$. Using (B9), we have that $1/M = dP/d\lambda^2$. Hence in the present case, $M = 1$. Now the required transforms are

$$\begin{aligned}
 \mathcal{K}'(0) &= \int_0^\infty (-\lambda)e^{-\lambda \cdot 0} k(\lambda) d\lambda \equiv -\frac{1}{2}MS_c^2 \\
 \mathcal{K}(0) &= \int_0^\infty e^{-\lambda \cdot 0} k(\lambda) d\lambda = \int \frac{dm}{d\lambda^2} \frac{d\lambda}{MS_c^2} MS_c^2 = \int_0^\infty \frac{dP}{d\lambda^2} d\lambda MS_c^2
 \end{aligned}$$

so that (B10) becomes

$$\omega = \frac{1}{2}M - \frac{1}{4}M^2 \left[\int_0^\infty (dP/d\lambda^2) d\lambda \right]^2$$

Now using the appropriate algebraic forms of $P(\lambda^2)$ to evaluate [...], we obtain $\omega = 0.32$.

APPENDIX C. FRACTION OF PHYSICAL LINKS AVAILABLE FOR HOPPING

We are working in the direct lattice with sites all having the same radius. We can work with a representative site having an inclusive figure (IF) radius R_c at the onset of percolation. The mean number of physical links is simply $\pi R_c^2 n_s \approx 4(R_c/2r_s)^2$. Not all of these links can lead to conduction, because the probability of hopping is

$$\exp(-\xi) = \exp(-2\alpha r - \Delta E/kT)$$

and in the percolation approximation, all links with $\xi < \xi_c$ conduct, while links with $\xi > \xi_c$ cannot. Only links with small energy jumps ΔE such that

$$\Delta E/kT < \Delta E_{\max}/kT = \xi_c - 2\alpha r$$

are involved in conduction, and this limit varies with radius. Between radii r and $r + dr$ we have $2\pi r n_s dr$ sites that overlap with the representative site. We calculate the fraction y of such links that can conduct, assuming a simple model of an impurity band extending between $\pm W$ from the Fermi level and having a constant density of states $N = n_s/2W$. Then there are two possible conditions:

$$\begin{aligned} y &= 1, & r < r_a \\ y &= 2N \Delta E_{\max}/n_s = (kT/W)(\xi_c - 2\alpha r), & r > r_a \end{aligned}$$

where

$$\begin{aligned} \xi_c - W/kT &= 2\alpha r_a \\ \xi_c &= 2\alpha R_c \end{aligned}$$

At high temperature, $kT \rightarrow \infty$, $r_a \rightarrow R_c$ and the mean value of y becomes $\bar{y} = 1$. All physical overlaps form conductive links, and we have the r -percolation limit. At lower temperatures, we have

$$\begin{aligned} \bar{y} &= \left[\int_0^{r_a} 2\pi r n_s dr + \int_{r_a}^{R_c} (kT/W)(\xi_c - 2\alpha r) 2\pi r n_s dr \right] \\ &\quad \times \left(\int_0^{R_c} 2\pi r n_s dr \right)^{-1} \\ &= 1 - (W/kT\xi_c) + (W/kT\xi_c)^2/3 \quad \text{for } kT\xi_c/W > 1 \end{aligned}$$

At still lower temperatures, the parameter r_a becomes negative. This implies that some physical links do not conduct even at small separations. Under these conditions, the limit r_a must be changed to zero in the integrals, with the result

$$\bar{y} = kT\xi_c/3W \quad \text{for } kT\xi_c/W < 1$$

The position at which this result takes effect is marked with an arrow in Fig. 4. It is clear that virtually the whole of the temperature variation of conductivity comes from this region.

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