Conduction in Random Systems*

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(Received 9 April 1973)

We have calculated numerically the conductivity of a system of random points connected by conductances that decrease exponentially with the separation distance. We compare critically various methods that have been proposed to solve the problem of hopping conduction in amorphous semiconductors and observe that the numerical results can be quantitatively understood using ideas based on percolation theory.

I. INTRODUCTION

There has been considerable recent interest in the problem of electrical conduction in amorphous semiconductors. A model for the material, which has been widely used as the starting point for calculations of the conductivity, was proposed by Mott[1] and used by him to predict the empirically successful formula

$$\sigma = \sigma_0 e^{-(T_0/T)^{1/4}} . \tag{1.1}$$

In the model, charge is assumed to be transported by the hopping of electrons between localized states that are randomly distributed in position and energy. The essential difficulty that has plagued all attempts to improve upon Mott's treatment of his model is precisely this randomness, which cannot be dealt with by reaching into some standard bag of mathematical tricks. Thus, although several investigators[2-4] have published what are claimed to be more systematic justifications of Eq. (1.1), every derivation contains more or less uncontrolled approximations and there are large differences from one treatment to the next in the relationships obtained between the quantities σ_0 and T_0, and the microscopic parameters of the model.

In this paper we attempt to arbitrate between the various calculational schemes alluded to above by the use of numerical methods. Previous numerical studies[5] related to this problem have appeared. None of them, however, incorporates the random nature of the hopping, which we consider to be the essential feature of the problem and have insisted on retaining. On the other hand, in the interest of numerical conclusiveness we have been willing to make other simplifying assumptions. Thus, to keep the computations manageable, we have omitted the energy dimension from the conductances g_{ij} associated, through arguments given originally by Miller and Abrahams,[6] with every pair of sites in Mott's model:

$$g_{ij} = \frac{e^2}{kT}\,\gamma_0 e^{-\alpha r_{ij} - (|E_i| + |E_j| + |E_i - E_j|)/2kT} , \tag{1.2}$$

where the sites are separated by the distance r_{ij}, and E_i and E_j are their energies. This simplification does not compromise the comparison we wish to make, as all theoretical methods of interest can still be applied, and they again lead to predictions which differ widely from one another.

In our model, then, we consider a number N (~ 1000) of random points enclosed in a cube and periodically extended in all directions. The points are connected by conductances g_{ij}, which depend on the separating distances according to the relation $e^{-\alpha r_{ij}}$. With the aid of a computer we calculate the current through this system when a voltage is periodically applied across it, i.e., each point and its forward periodic image in the z direction are maintained at a potential difference U_0. A comparison of our results with various predictions is given in the following sections. In brief, our computations show that the conductivity of the model system has a leading exponential dependence of the form $e^{-\alpha r_c}$, where r_c is a number well explained by the ideas based on percolation theory developed in Ref. 2. As applied to the present model, these ideas require r_c to be the separation distance up to which pairs of the randomly distributed points would have to be connected to obtain a nonzero probability of a cluster of connected points extending across the system. Holcomb and Rehr[7] have studied precisely this question and have found that such a system has a "percolation threshold," defined in the preceding sentence, when 0.30 points on the average are enclosed in a sphere of radius $r_c/2$, i.e., $p_c = (N/V)\frac{4}{3}\pi(r_c/2)^3 = 0.30$, N/V being the density of points. Our value for r_c obtained from the conductivity agrees well with this formula. Thus, in retrospect, it appears that we have provided a method for obtaining the threshold for percolation in a random system.

We also had the aim of learning something about the nonexponential prefactor of the conductivity. In this we failed because of inherent limitations in the numerical approach. Thus, from our numerical study per se, we have nothing to say about the

prefactor, although some general thoughts on this subject are given in Sec. II and in an appendix.

In Sec. II of this paper we present our results and discuss their accuracy and their relation to percolation. Sec. III contains a critique of the different theories in light of the numerical results. Finally, there are four appendixes: Appendix A deals with the details of our numerical algorithm; Appendix B, the derivation of the predictions of the method of Brenig *et al.*[4] applied to our model; Appendix C, the nonexponential prefactor; and Appendix D, a commonly used random-number generator which we found afflicted with a significant, albeit mild, correlation.

II. NUMERICAL RESULTS AND DISCUSSION

We began with N randomly distributed points in a cube of unit volume and their periodic extensions. Each pair (ij) of points was, in principle, connected with conductances of the form

$$g_{ij} = g_0 e^{-\alpha r_{ij}} \tag{2.1}$$

and α was allowed to vary. The conductivity of the system was computed by assigning voltages to each site and solving the network equations iteratively, insisting that there be a potential difference U_0 between every point and its next periodic image in the z direction. [We discuss this technique in more detail in Appendix A.] From the potentials so obtained we computed the current crossing a face of the cube perpendicular to the z direction.

We chose to work with systems of $N = 2000$, $N = 1000$, $N = 500$, and $N = 200$. The results are given in Fig. 1. Figure 1 shows the current as a function of $\alpha/\rho^{1/3}$ (where ρ is the density of points). Here, for practical reasons, only about eight nearest neighbors have been linked by the conductances (2.1). This completely warps the picture for small α, where the conductance must increase without bound as N is increased with all pairs linked. For large α, however, the results are unchanged as all neighbors up to a given distance have been included and the long links become extremely weak.

A remarkable property of the plot of $\log_{10} I$ vs $\alpha/\rho^{1/3}$ in Fig. 1 (where I is the current in units of $g_0 U_0$) is that all the asymptotes at large $\alpha/\rho^{1/3}$ intersect the line $\alpha = 0$ at $\log_{10} I = 0$. After observing this feature it is possible to understand it. As α grows larger and larger, the potential difference must all concentrate on one single conductance in the cube. The current will choose the path in which the longest hop is as short as possible because all other paths will become infinitely worse as α grows. For the same reason all the other conductors along this chain will finally become infinitely better and all the potential difference will become concentrated on the weakest link of the best chain. In the limit $\alpha \to \infty$ the current will thus behave like

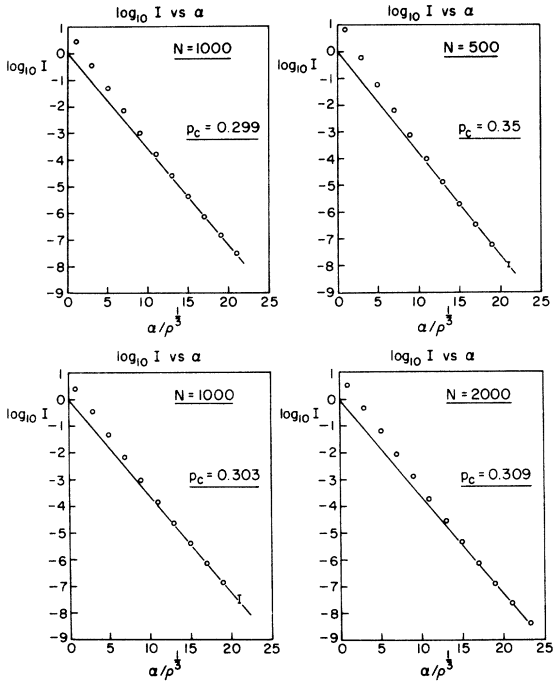

FIG. 1. Logarithm of the current I, in units of $g_0 U_0$, vs $\alpha/\rho^{1/3}$ for several systems of 500, 1000, or 2000 nodes. The percolation threshold p_c is calculated from the slope of the asymptote.

$$I = e^{-\alpha r_c}, \tag{2.2}$$

where r_c is the longest hop in the best chain. It is clear that the logarithm of the asymptotic form, Eq. (2.2), if extrapolated to $\alpha = 0$, will intersect this line at $\log_{10} I = 0$. It is also clear from the above discussion, and the line of argument given in the Introduction, that r_c is the distance up to which points must be connected for percolation in the *finite* systems we are considering. One is naturally led to ask how much the value of r_c is influenced by the finiteness of the model systems. Empirically we found that we could not discern any systematic variation in $p_c \equiv (N/V)\frac{4}{3}\pi(r_c/2)^3$ between our networks with $N = 1000$ and $N = 2000$, though p_c seemed to increase slightly as N was lowered to 500 and 200. A systematic extrapolation to bigger N turned out to be difficult. For small N the scatter from one array to the next was large, and obtaining a true ensemble average would have been prohibitively expensive in computer time. In the case of the $N = 1000$ arrays, of which we tried three, although the scatter in p_c from one to the next seemed smaller, we were limited in accuracy by the imperfect convergence of our numerical procedure at large α. Thus all we can say with confidence is that the large-N limit of p_c determined by this method is $p_c = 0.30 \pm 0.015$. As we have al-

ready remarked this result agrees well with another calculation of the percolation threshold in a random system.[7]

Some further discussion is needed to relate the results of these computations to the thermodynamic limit of the conductivity of a large system. One may understand how to pass to this limit by realizing that increasing N at fixed $\alpha/\rho^{1/3}$ and fixed volume is, by a change in the scale of lengths, equivalent to increasing the volume at fixed density. More precisely, if one views the calculation as determining the ensemble average of the dimensionless conductance I (i.e., the current through the system divided by g_0U_0) as a function of the three variables $\alpha/\rho^{1/3}$, N, and V (the volume of the box), scale invariance implies that

$$I(\alpha/\rho^{1/3}, N, V) = I[(\alpha/\lambda^{1/3})(\rho/\lambda)^{-1/3}, N, \lambda V] = I(\alpha/\rho^{1/3}, N, \lambda V) , \quad (2.3)$$

where λ is an arbitrary scaling parameter. [Equation (2.3) simply says that increasing the separation of the sites, keeping the number of sites fixed but at the same time changing the length $1/\alpha$ over which the conductance (2.1) varies, does not change the impedance of the system.] In calculating the thermodynamic limit one requires N and V to increase proportionately. Thus the thermodynamic limit of the conductivity σ_{th} corresponding to a density ρ is given by

$$\sigma_{th}(\rho, \alpha/\rho^{1/3}) = \lim_{N\to\infty} (\rho/N)^{1/3} g_0 I(\alpha/\rho^{1/3}, N, N/\rho) . \quad (2.4)$$

By the change of scale (2.3) we may relate the terms of the sequence in (2.4) to the calculations at fixed (unit) volume that we have done. Thus

$$\sigma_{th}(\rho, \alpha/\rho^{1/3}) = \lim_{N\to\infty} (\rho/N)^{1/3} g_0 I(\alpha/\rho^{1/3}, N, 1) . \quad (2.5)$$

Examining a term in the sequence in Eq. (2.5) for large but fixed N shows now that the asymptote (at $\alpha \to \infty$) of the logarithm of the conductivity intersects the line $\alpha = 0$ at $\log_{10}(g_0 \rho^{1/3}/N^{1/3})$, i.e., lower down for larger N. On the other hand, one would certainly expect, as discussed above, that the slope of the asymptotic curve would become infinitesimally smaller as V increases because incipient percolation should be slightly easier in a larger system. However, for small α the different terms in the sequence for σ must lie on top of each other. Finally, one expects σ_{th} to stay above each term in the sequence when $\alpha \to \infty$ because, for finite N, the current paths are always limited. These observations suggest that in the thermodynamic limit $\log\sigma_{th}$ will not have a straight line asymptote as $\alpha \to \infty$ but a continuous curvature. A possible form would be

$$\sigma_{th} \propto g_0 \rho^{1/3} (1/\alpha r_c)^{\nu} e^{-\alpha r_c} \quad \nu > 0 . \quad (2.6)$$

Indeed (2.6) can be made consistent with (2.5) by interpreting the thermodynamic-limit curve as approaching the support curve formed by the successive asymptotes in the sequence (2.5). Making this assumption r_c can be shown to vary as $r_c(N) = r_c(\infty) + (\text{const}) \times (N)^{-1/3\nu}$. From this consideration and our few runs with N smaller than 1000 we conclude that $\nu < 1$.

To test whether the nonasymptotic part of our calculations contained any information about the preexponential factor, we ran a system in which we kept track of 16 nearest neighbors instead of 8. We found that this altered the calculated I for $\alpha/\rho^{1/3} < 9$. Examination of Fig. 1 shows that for $\alpha/\rho^{1/3} > 9$ one is already very close to the straight-line asymptote. This indicates that information about the power ν in (2.6) is not contained in the curves of Fig. 1.

In spite of the limitations of these calculations, which we have emphasized, the result that emerges forcefully is that the leading exponential behavior is given by the percolation threshold. Any theory which does not give this dependence correctly cannot be trusted to give information about the nonexponential prefactor.

III. COMPARISON WITH THEORIES

Here we summarize the predictions that various methods which have been used to analyze the hopping conduction problem would give for our model.

A. Percolation Theory

There is little need to say more on this approach, which we have had to discuss extensively in Sec. II in presenting the results of our computations, except to discuss approximate methods for calculating the percolation threshold. We have relied on the numerical agreement of our results and the computation of Holcomb and Rehr.[7] Obviously, it would be satisfying if some analytical progress could be made.

(i) *Effective-medium theory.*[8] In this method one imagines embedding conducting and nonconducting spheres in an otherwise uniform virtual material whose conductivity is such that the net effect of the two types of embedded particles provides no change of resistance. The result of the calculation is $\sigma \propto (p - \frac{1}{3})$, i.e., one finds $p_c = 0.33$.

(ii) *Pollak's method.*[3] Accepting as his starting point the idea of percolation, Pollak tries to set up a formalism to actually calculate the percolation threshold for which he obtains a lower bound. He then treats the essential quantity, equivalent to $8p_c$, as a parameter. Instead of 2.4 he estimates this to be equal to 1.7, obtaining the result quoted in Table I.

TABLE I. Results.

	r_c/r_s	p_c	preexponential
Percolation (our results)	1.34	0.30	$(1/\alpha r_c)^\nu$, $\nu > 0$
Effective medium	1.38	0.33	
Pollak	1.19	0.21	
Brenig *et al.*	0.89	0.087	α^0
Fibich and Ron	$(\frac{1}{2}\alpha r_s)^{1/2}$ $\left[r_s = \left(\frac{4\pi}{3}\rho\right)^{-1/3}\right]$		

B. Theory of Brenig *et al.* (Refs. 4 and 9)

In this method the problem is reduced, making general and plausible assumptions, to the problem of calculating the velocity of sound of a random harmonic crystal with, however, force constants that depend exponentially on the separations. The details of this method and the application to the model of the present paper are given in Appendix B. The result is of the form

$$\sigma = \sigma_0 e^{-\alpha \bar{r}_c} , \tag{3.1}$$

where

$$\bar{p}_c = (N/V)\tfrac{4}{3}\pi(\bar{r}_c/2)^3 = 0.087 .$$

As shown in Appendix B, the method is expected to give an upper bound to the conductivity. The discrepancy between $\bar{r}_c$ and the correct percolation value r_c is so large as to render the bound meaningless. Brenig *et al.* also attempt to calculate the prefactor σ_0 in (3.1). The lowest upper bound one can obtain by this method predicts a σ_0 which has no α dependence. The arguments given in Sec. II lead us to doubt that this can be correct. Unfortunately, therefore, although the method strikes us as being elegant and ingenious, it seems to have little quantitative value.

C. Method of the Most Probable Value

Ron and Fibich[10] have recently suggested that in the Mott model one obtains the correct result by considering the probability distributions of the conductances between neighbors, and taking the required conductivity to be proportional to the most probable value of these conductances. This hypothesis leads to a functional form different from (1); viz., it leads to the form $\sigma_0 e^{-(T_0/T)^{1/3}}$. Applied to our model, the hypothesis predicts $\sigma \propto e^{-\alpha^{3/2}(4\pi\rho)^{-1/2}}$. In the large-$\alpha$ region, $\alpha^3 \gg \rho$, this result predicts a much smaller conductivity than given by the percolation threshold. The error in this method lies in the fact that if each link is optimized without regard to the over-all conductivity of a chain of links, then one will not avoid dead ends from which there is no exit except by means of a link of very low conductance. Our computer experiments rule out the dependence predicted by this method.

The results of the methods discussed above are summarized in Table I.

ACKNOWLEDGMENTS

It is a pleasure to acknowledge discussions with M. Fisher, B. Halperin, B. Nickel, T. Padmore, J. Rehr, and P. Wölfle.

APPENDIX A

To solve for the potentials of the N nodes we used a Gauss–Seidel[11] iteration procedure in standard or over-relaxed form. In the context of our problem this corresponds to calculating a potential for each site according to Kirchhoff's rule,

$$V = \sum_j (V_j/R_{ij}) \Big/ \sum_j (R_{ij})^{-1} , \tag{A1}$$

and setting the new potential at that site equal to

$$V_i^{(n+1)} = V_i^{(n)} + w(V - V_i^{(n)}) , \tag{A2}$$

where $V_i^{(n)}$ refers to the potential of the ith site after the nth iteration, R_{ij} is the resistance between sites i and j, and w is the over-relaxation parameter $(1 < \omega < 2)$. In each iteration all the potentials are set to new values using as the potentials of the neighboring points the instantaneous values irrespective of whether they date from the previous iteration or have been changed in the course of the current one. We carried out the iteration in the original (random) numbering sequence of the nodes always in the same direction or back and forth, with no perceptible difference in the rate of convergence. It seems from our experience that a large $w(\sim 1.6)$ is advantageous at relatively low values of the parameter α $(\alpha/\rho^{1/3} < 15)$. As one would superficially expect from the general criteria for determining w, at large α the optimum value of w approaches unity.

It is easy to understand that the case of large α presents the convergence problem of long paths of low resistance with a dead end or large regions of equal potential connected only at a single point to a real current-carrying path. For large enough α this completely wrecks the method in the form we used it as we found no simple way of eliminating the dangling paths or areas.

We started the iteration with the obvious guess

$$(E_0 = U_0/\text{length})\ V_i^{(0)} = -E_0 z_i$$

and took the previous potentials each time we increased α. At the end we calculated the current through several successive cross sections of the cube for an estimation of accuracy after termina-

ting the iteration on a criterion that the average absolute change in the voltages be smaller than a set limit.

It generally turned out that if convergence was not reached in about 300 interactions, subsequent progress was extremely slow.

APPENDIX B

In the following we summarize the application of the methods of Brenig *et al.*[4] to our problem. What we seek, and what the computer program simulates, is a time independent solution to the equation ($E_0 = U_0/\text{length}$)

$$C_i \frac{d}{dt}\,\delta V_i = -E_0 \sum_j G_{ij}(z_i - z_i) + \sum_j G_{ij}(\delta V_j - \delta V_i)\ . \tag{B1}$$

Above, we have written the potential at site i as $V_i = -E_0 z_i + \delta V_i$. The periodic boundary condition requires that if $i+N$ labels a repetition of the site i then

$$\delta V_{i+N} = \delta V_i\ . \tag{B2}$$

[The constants C_i, formally capacitances, have been chosen in the computer calculation to facilitate convergence.] Equation (B1) can be put in correspondence with the kinetic equation [Eqs. (1) and (7)] of Ref. 4, called BDW in this appendix. By following the analysis of Sec. 3 or Appendix A of BDW one obtains the formula

$$\sigma = +\frac{1}{V}\lim_{k\to 0}\frac{1}{k^2}\sum_\rho |\ (e^{ikz})_\rho\ |^2 \gamma^\rho\ , \tag{B3}$$

where ρ refers to the eigenvalue equation

$$\sum_j{}' G_{ij}(u_i^\rho - u_j^\rho) = \gamma^\rho C_i u_i^\rho\ . \tag{B4}$$

Here the prime on the summation symbol means that the sum is only over one periodicity volume. The eigenvectors u_i are normalized according to

$$\sum_i (u_i^\rho)^* C_i u_i^\sigma = \delta_{\rho\sigma} \tag{B5}$$

and the expansion coefficients $(e^{ikz})_\rho$ are defined by

$$e^{ikz_i} = \sum_\rho (e^{ikz})_\rho u_i^\rho\ . \tag{B6}$$

Equation (B3) casts the problem into an extremely elegant form, but it is evident that further analytical progress is likely to be difficult. Indeed, we shall show that the very ingenious approximation schemes invented by Brenig and co-workers are quantitatively not very successful. In the following we shall give a slightly modified version of these approximations which shows that they give a result which is likely to overestimate the conductivity. From our numerical work we have seen that this is the case, and the amount of the overestimate has been discussed in the main text of this paper.

The attempt is to calculate the logarithm of the eigenvalue in Eq. (B3). This is facilitated by introducing as a mathematical device a parameter λ in the following way. Replace the conductances $G_{ij} = G_0 e^{-\alpha r_{ij}}$ by $G_{ij}(\lambda) = G_0 e^{-\lambda\alpha r_{ij}}$. Then one has

$$\frac{1}{\gamma^\rho}\frac{\partial\gamma^\rho}{\partial\lambda} = -\frac{1}{2\gamma^\rho}\sum_{ij} s_{ij} G_{ij}\,|\,u_i^\rho - u_j^\rho\,|^2 < -\sum_i s_{i\bar{i}} P_i^\rho\ , \tag{B7}$$

where we have written $s_{ij} = \alpha r_{ij}$, $\bar{i}$ refers to the nearest neighbor of the site i, and the real positive quantity P_i^ρ is evidently

$$P_i^\rho = \frac{1}{2\gamma^\rho}\sum_j G_{ij}\,|\,u_i^\rho - u_j^\rho\,|^2\ . \tag{B8}$$

[Note that $\sum_i P_i^\rho = 1$.] After some simple manipulations in which the reality of P_i^ρ, G_{ij}, C_i, and γ^ρ are useful one can write

$$P_i^\rho = P_i^{\rho(1)} + P_i^{\rho(2)}\ , \tag{B9}$$

where

$$P_i^{\rho(1)} = C_i\,|\,u_i^\rho\,|^2 \tag{B10}$$

and

$$P_i^{\rho(2)} = \frac{1}{2\gamma^\rho}\sum_j G_{ij}(\,|\,u_j^\rho\,|^2 - |\,u_i^\rho\,|^2)\ . \tag{B11}$$

We note that

$$\sum_i P_i^{\rho(2)} = 0\ . \tag{B12}$$

Further, using an obvious symmetry,

$$\sum_i s_{i\bar{i}} P_i^{\rho(2)} = \frac{1}{2\gamma^\rho}\sum_{ij}(s_{i\bar{i}} - s_{ij})\,G_{ij}(\,|\,u_j^\rho\,|^2 - |\,u_i^\rho\,|^2)\ , \tag{B13}$$

which shows that the largest G_{ij}, namely $G_{i\bar{i}}$, makes no contribution to the $P^{(2)}$ part of the upper bound in (B7). We also note that for a regular array of sites $P_i^{(2)} \equiv 0$. These observations suggest but do not prove that in the low-density limit $n \ll \alpha^3$ one may neglect $P^{(2)}$. The remaining term is in fact the BDW approximation to the first expression in (B7). The approximate expression is then evaluated by taking for the eigenfunctions in question the long-wavelength limit

$$u_i = \left(\sum_i C_i\right)^{-1/2} e^{ikz_i}\ . \tag{B14}$$

Using this form in (B10) and (B7) one then finds

$$\frac{1}{\gamma}\frac{\partial\gamma}{\partial\lambda} < -\frac{1}{N}\sum_i s_{i\bar{i}}\ , \tag{B15}$$

where N is the number of sites in the periodicity volume. [For lack of a better symbol we have used an inequality sign in (B15).] The right side of (B15) is independent of G_{ij} (and thus λ) and is easily evaluated by using the Poisson distribution. The result is that the exponential dependence of the conductivity is given as $e^{-\alpha r_{\min}}$, where $r_{\min} = (3/4\pi\rho)^{1/3}$

$\times\Gamma(\frac{4}{3})$. This value has been discussed in the main text.

It is instructive to use our model to discuss a calculation of the preexponential factor by Brenig and co-workers. This calculation proceeds by writing the identity

$$\gamma(\lambda=1)=\gamma(\lambda)\exp\int_{\lambda}^{1}d\lambda'\,\frac{1}{\gamma(\lambda')}\,\frac{\partial}{\partial\lambda'}\,\gamma(\lambda')\,, \qquad \text{(B16)}$$

using (B15) to evaluate the exponential factor and a straightforward variational estimate for $\gamma(\lambda)$ based on the trial function (B14). The value for $\gamma(\lambda)$ is thus clearly an upper bound, but it is expected to be most successful when λ is small, i.e., when $(\alpha\lambda)^{-1}$ is large. Carrying out this calculation one finds from (B3)

$$\sigma<\frac{4\pi(4!)}{6}\,G_0\,\frac{\rho^2}{(\alpha\lambda)^5}\,e^{-(1-\lambda)\alpha r_{\min}}\,. \qquad \text{(B17)}$$

The inequality has to be qualified as indicated below (B15). In all the above work λ has not had to be specified very precisely. In Ref. 10 the preexponential factor quoted is obtained[12] by an operation equivalent to setting $\lambda\alpha r_{\min}=1$. On the other hand (B17) would suggest varying λ to minimize the right-hand side, which would lead to $\lambda\alpha r_{\min}=5$, and reduce the preexponential factor by more than two orders of magnitude. This sensitivity of the approximation scheme to the joining point seems to us a dangerous sign. We are, as mentioned in the main text above, skeptical of both the functional dependence and the numerical value of preexponential factors obtained by this method.

APPENDIX C

In this appendix scaling arguments will be suggested which give plausible bounds to the power ν of the nonexponential prefactor in Eq. (2.6). The full four-dimensional problem incorporating the energies of the sites will briefly be discussed at the end.

The scaling argument hinges on the observation that there will be a smaller and smaller density of links which carry an appreciable current and have a large potential step across them as α grows larger. These power dissipating links will be called active in the following. Their lengths are distributed over a small increment of order $1/\alpha$ around r_c, as larger links are very bad and shorter links very good conductors compared with the critical links for percolation. Some active links are shorter than r_c, as they have not yet, at a given α, become essentially perfect conductors compared with the critical links and, conversely, some active links are larger than r_c. It is not clear whether the distribution is centered at exactly r_c.

Imagine now α multiplied by some factor m. Roughly the fraction $1/m$ of the former active links will remain in the range where they can qualify as active. If they actually did qualify, scaling up the volume by the same factor would produce a system where the number of active links would be unchanged. Assuming that the general topology of the islands of constant potential between the active links would not change drastically, this would lead to a system of the same *impedance*, apart from the exponential factor, and therefore to a conductivity scaled down by an inverse length of $m^{-1/3}$.

The scaling argument in the above form rests on three assumptions: The active links decrease exactly as α^{-1}, the general topology of the system is invariant to scaling, and the exponential variation does not introduce additional powers of α. The first assumption is clearly not strictly correct. All former active links will not qualify in the new system. A link longer than r_c, when it falls outside the domain of those active, can sever a whole path of current and render a host of other links useless. Also a link shorter than r_c can short out a formerly active parallel conductor. Therefore the number of real active links will decrease faster than $1/\alpha$, and the conductivity correspondingly faster than $(1/\alpha)^{1/3}$, i.e., $\nu\geq\frac{1}{3}$. The remaining two assumptions in the argument are the equality of the general topology, which although plausible cannot be rigorously justified, and the tacit assertion that the exponential factor will not change anything. If the distribution of the active links is not exactly centered on r_c, the exponential factor will be of the form

$$e^{-\alpha(r_c)+A/\alpha+O(1/\alpha^2)}\approx e^{-\alpha r_c}e^{A+O(1/\alpha)}$$
$$\approx e^{-\alpha r_c}e^{A}[1+O(1/\alpha)]$$

and this will not alter the argument. We therefore conclude that $\nu\geq\frac{1}{3}$ based on the assumption that the general shape of the regions of constant potential will not change in the process of scaling.

Consider now the full four-dimensional problem of Eq. (1.2). Proceeding according to Ref. 2 we can say that smaller conductors than those just needed for percolation contribute little and we write for the conductors that do contribute

$$\alpha R_{ij}+(\,|E_i|+|E_j|+|E_i-E_j|\,)/2kT<\ln(\gamma_0/\Gamma_c)\,, \qquad \text{(C1)}$$

where $\Gamma_c=kTG_c/e^2$ and G_c is the critical conductance for percolation. In dimensionless form

$$\frac{R_{ij}}{R_{\max}}+\frac{|E_i|+|E_j|+|E_i-E_j|}{2E_{\max}}<1\,, \qquad \text{(C2)}$$

where

$$R_{\max}=(1/\alpha)\ln(\gamma_0/\Gamma_c)\,, \qquad \text{(C3)}$$

$$E_{\max}=kT\ln(\gamma_0/\Gamma_c)\,. \qquad \text{(C4)}$$

The conductivity varies as $e^{-(T_0/T)^{1/4}}$ or $\ln(\gamma_0/\Gamma_c)$

varies as $T^{-1/4}$. Therefore, from Eq. (C3), R_{max} varies also as $T^{-1/4}$ and E_{max} as $T^{3/4}$. The percolation criterion can be expressed as

$$(2\rho_0 E_{max}) R_{max}^3 = \nu_c \,, \tag{C5}$$

where ρ_0 is the density of states per unit energy and volume and ν_c a dimensionless constant. The criterion remains satisfied at all temperatures, with the quantities in it varying as described above.

When the temperature is lowered by a factor m the energy range $\sim (kT)^{3/4}$ of the active traps is narrowed or the spatial density of active traps is lowered by the factor $(1/m)^{3/4}$. Again the spatially equivalent situation can be recovered by looking at a larger volume by $m^{3/4}$. By the same argument as in the three-dimensional case the conductivity will then carry the factor $T^{1/4}$ apart from the exponential variation.

The above discussion is equivalent to taking into account the geometrical factor $\rho^{1/3}$ in Eq. (2.6) for the conductivity since a real reduction in the density of active traps has taken place. In fact Eq. (2.6) suggests that the reduction of the density should lead to an even higher power of T in front of the expression, since the prefactor $(1/r_c\alpha)^{\nu}$ depends on ρ as $\rho^{\nu/3}$, or on T as $T^{\nu/4}$. However, this last point should be discussed in the full four-dimensional case. Through making use of the dependences of R_{max} and E_{max} on the temperature, the four-dimensional exponential factor can be written as

$$\sigma \propto e^{-S_{max}/T^{1/4}} \,, \tag{C6}$$

where

$$S_{max} = \alpha R_{max}(T_0)\, T_0^{1/4} = (1/k) E_{max}(T_0)\, T_0^{-3/4} \tag{C7}$$

is a distance in the four-dimensional space, where one keeps looking at a larger and larger volume and smaller and smaller energy range when T grows smaller compared with some arbitrary reference T_0. By analogy with Eq. (2.6) one expects a nonexponential prefactor of the form $(T^{1/4}/S_{max})^{\nu'}$, $\nu' > 0$. Together with the power $\frac{1}{4}$ of T this gives a prefactor $T^{(1+\nu')/4}$. Not knowing ν' we may conclude that there is a positive power of T larger than or equal to $\frac{1}{4}$ in the prefactor of the full four-dimensional case. The inverse power of T in the factor e^2/kT of Eq. (1.2) will of course also carry over to the conductivity.

APPENDIX D

We found a subtle systematic correlation in the IBM-360/65 random number generator RANDU:

$IX = IX * 65539 \quad (65539 = 2^{16} + 3)$

$IF(IX)\,1, 2, 2$

1 $IX = IX + 2147483647 + 1$

2 $RAN = IX + 4.656612E - 10 \quad (0 < RAN < 1)$.

In one computation we kept track of nearest neighbors of nodes up to a given radius, which for $N = 1000$ we chose such that each node would be connected, on the average, to 8.15 correspondents. We then generated the x, y, and z coordinates of the first node, the x, y, and z of the second, and so on, in this order, with RANDU up to 1000 nodes. With five different seeds (the first IX's specified by us) we counted 8.56 nearest neighbors on the average, with a variance of $\sigma = 0.06$, enclosed in spheres of the chosen radius centered on each node. Changing the number of nodes or the radius always lead to a similar result: The mean number of nearest neighbors was systematically several standard deviations (when the seed was varied) smaller or larger than the exact statistical result.

We therefore used a more complicated procedure, suggested by Nickel,[13] to generate our random numbers which passed the above test. We first composed a table of 256 RANDU numbers and then picked our random numbers from this table with the aid of a similar generator (with the multiplier $= 2^{15} + 3$) to give us a random index varying from 1 to 256. Finally we replaced the number we picked with a new RANDU number. In this way we destroyed the correlation between the nth and the $(n+3)rd$ RANDU numbers.

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*Work supported in part by the U. S. Office of Naval Research under contract No. N00014-67-A-0077-0010, Technical Report No. 34, and by the National Science Foundation, Grant No. GH-33637, through the Materials Science Center at Cornell University, MSC Report No. 1980.

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[1]N. F. Mott, Philos. Mag. **19**, 835 (1969).

[2]V. Ambegaokar, B. I. Halperin, and J. S. Langer, Phys. Rev. B **4**, 2612 (1971).

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

[4]W. Brenig, G. Döhler, and P. Wölfle, Z. Phys. **246**, 1 (1971).

[5]S. Kirkpatrick, Phys. Rev. Lett. 27, 1722 (1971); B. J. Last and D. J. Thouless, Phys. Rev. Lett. 27, 1719 (1971); D. Adler, L. P. Flora, and S. D. Senturia, Solid State Commun. 12, 9 (1973).

[6]A. Miller and E. Abrahams, Phys. Rev. **120**, 745 (1960).

[7]D. F. Holcomb and J. J. Rehr, Jr., Phys. Rev. **183**, 773 (1969). Their result $p_c = 0.29$ agrees very well with ours and an extrapolation to the continuum limit (private communication) makes the two equal, $p_c = 0.30$. In spite of an unfortunate wording the definition of p_c by these authors, misinterpreted by V. K. S. Shante and S. Kirkpatrick [Adv. Phys. **20**, 325 (1971)], coincides with ours.

[8]D. A. G. Bruggeman, Ann. Phys. (Leipz.) **24**, 636 (1935); R. Landauer, J. Appl. Phys. 23, 779 (1952) and footnote 31 of Ref. 2.

[9]W. Brenig, G. Döhler, P. Wölfle (report of work prior to publication).

[10]M. Fibich and A. Ron, Solid State Commun. 11, 1509 (1972).

[11]See, e.g., E. Issacson and H. B. Keller, *Analysis of Numerical Methods*, (Wiley, New York, 1966).

[12]P. Wölfle (private communication).

[13]B. Nickel (private communication).