Classical Transport in Disordered Media: Scaling and Effective-Medium Theories*

Scott Kirkpatrick†
James Franck Institute, The University of Chicago, Chicago, Illinois 60637
(Received 1 September 1971)

Electrical conduction in resistor networks with all but a fraction p of the resistors removed is studied as a paradigm of classical transport in disordered materials. A self-consistent effective-medium theory provides a quantitative description of the model, except in a small critical region, where the scaling law $\sigma \propto (p-p_c)^{8/5}$ is satisfied (in three dimensions), with p_c the critical probability for bond percolation. It is also contrasted with a critical-path analysis recently developed for the study of hopping conduction.

Classical limits have been invoked recently for the study of electronic conduction in disordered materials by authors[1,2] interested variously in extended states just above a mobility edge,[3] or hopping conduction among localized states well below.[4,5] This Letter reports three new results relating to the classical transport problems defined in these limits:

(1) The conductivity of a Monte Carlo sampling of disordered resistor networks has been computed in order to resolve some current speculation about classical transport near a percolation[6-8] threshold. The results obtained should also describe, by inference, the mobilities of the extended electronic states of a disordered system with energies close to that of a mobility edge.[3]

(2) An old effective-medium theory of conduction in mixtures[9] has been re-examined and generalized to treat resistor networks. It gives surprisingly accurate predictions of the observed results under a wide range of conditions.

(3) A very different point of view from that of (2) focuses not on the average properties of the medium, but on the details of the critical paths[4,5] along which much of the current must flow. This analysis can be applied to our networks as well, but the quantitative accuracy obtained, even in favorable cases, proves inferior to that possible with the effective-medium theory.

Several authors[1] recently have suggested that the transport properties of an electron with energy E near a mobility edge E_c, or the low-lying excitations of electrons in dense vapors,[2] could be studied semiclassically by calculating the conductivity of the region available for classically allowed motion with energy E in an appropriate random potential. If $p(E)$ is defined as the fraction of the volume which is allowed, a first approximation to the conductivity[1] is

$$\sigma(E) = \sigma_0 P(p(E)), \tag{1}$$

where $P(p)$, the percolation probability,[6-8] is the fraction of the volume allowed but not isolated, i.e., lying in infinitely extended channels; and σ_0 has a value characteristic of large allowed regions of the material. $P(p)$, sketched in Fig. 1, is known to vanish for p less than a critical value p_c, falls sharply to zero as $p \to p_c^+$, and tends to p as $p \to 1$. E_c is obtained from

$$p(E_c) = p_c. \tag{2}$$

A generalization of (1),

$$\sigma(E) = \mu(p(E))P(p(E)), \tag{3}$$

was introduced by Eggarter and Cohen[2] to take account of scattering off the boundaries of the allowed volume, but they argue that the effective mobility $\mu(p)$ is nonzero near p_c, so that the critical behavior of $\sigma(E)$ near E_c should be that of $P(p(E))$.

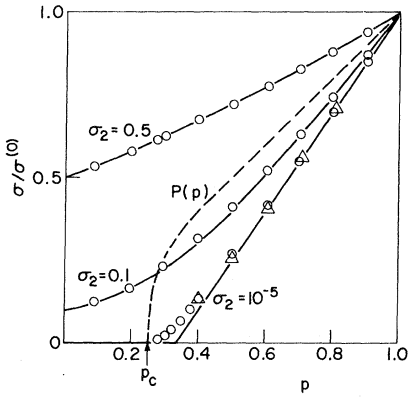

FIG. 1. Conductivity of a simple cubic network of conductances with binary disorder. Values of the conductances are 1 (with probability p) and $\sigma_2 < 1$ (probability $1-p$), assigned at random. Calculations for networks with $15\times15\times15$ nodes (data points) and predictions of the effective-medium theory described in the text (solid lines) are displayed for three values of σ_2 as labeled. p_c indicates the critical concentration for bond percolation on this lattice. The dashed line is proportional to $P(p)$ (Ref. 7) and represents the prediction of (1) for $\sigma_2 \ll 1$.

Last and Thouless,[10] however, have suggested that $\mu(p)$ may vanish at p_c because the rather constricted and convoluted shape of the first current-carrying regions to appear makes them inefficient conductors. The vanishing of $\mu(p_c)$ would weaken the critical behavior of $\sigma(E)$. This conjecture has been supported experimentally[10] by a measurement of the conductance of a piece of conducting paper with many small holes punched in it.

In order to remove the restriction to two dimensions (2D) inherent in the work of Ref. 10, and also to obtain a quantitative result, we have evaluated numerically the conductivities of large regular 2D square and 3D simple cubic networks, in which the values of the conductances (the bonds of the arrays) are chosen by a Monte Carlo procedure from one of several distributions. The voltages v_i at the nodes of each network, and from them the total current flow for a fixed external applied voltage, were obtained by a relaxation procedure based upon the Kirchhoff current law. If σ_{ij} is the conductance of the link between adjacent nodes i and j, the condition that all currents into node i cancel is

$$\sum_j \sigma_{ij}(v_i - v_j) = 0. \tag{4}$$

Resistor networks provide a convenient discrete model of a continuous medium whose conductivity varies with position. In fact, the network equation for currents, (4), is just the discrete form of the usual condition on a static current distribution, $\nabla \cdot \vec{j} = 0$. Also, the bond percolation properties of the arrays studied are accurately known ($p_c = \frac{1}{2}$ for a square, and $p_c = 0.25$ for a simple cubic lattice[8]), while the percolation properties of continuous regions are not.

Results obtained with a binary distribution of σ_{ij}, in which two values σ_1 and σ_2 occur with probabilities p and $(1-p)$, respectively, are shown in Figs. 1 (3D) and 2 (2D results). For each set of points, $\sigma_1 = 1$ and σ_2, taken to be less than σ_1, is indicated. The lowest sets of data in the two figures ($\sigma_2 = 10^{-5}$) are to be compared with the predictions of (1), (3), and Ref. 10. Like Last and Thouless,[10] we find that the critical behavior of σ near p_c is not that of $P(p)$ alone. In both 2D and 3D, σ appears to increase quite slowly just above p_c. The points in the "toe" of Fig. 1, for $p_c \leq p \leq 0.4$, were obtained from three different Monte Carlo samples, yet all satisfy the scaling relation

$$\sigma(p) \propto (p - p_c)^{8/5} \tag{5}$$

very closely. The exponent in (5) is accurate to at least ± 5%. No estimate of the scaling exponent in 2D could be made.

One immediate consequence of the scaling behavior (5) is an apparent softening of mobility edges. The $\sigma_2 = 10^{-5}$ data of Fig. 1 should be representative of the energy dependence of the mobility of states near the mobility edge in an amorphous semiconductor or chalcogenide glass, i.e., $\sigma(E) \propto (E - E_c)^{8/5}$ near E_c. This will give an activation energy for electronic conduction decreasing with temperature, as is generally observed in chalcogenide glasses.[11] The scaling behavior expressed in (5) may also be experimentally observable in photoconductivity measurements.

Effective-medium theory.—The straight-line portions of the data for $\sigma_2 \to 0$, in both Figs. 1 and 2, and all the points for which σ_1 and σ_2 were comparable can be accounted for by an old self-consistent effective-medium theory of conduction in mixtures.[9] The average effect of the random σ_{ij}'s can be expressed by giving all of them a single value σ_m, and choosing σ_m such that the effects of changing any one conductance back to its true value will, on the average, cancel out. The procedure is physically analogous to the construction of a "coherent potential"[12] in the theory of electrons in alloys.

Altering the value of a conductance aligned along the electric field from σ_m to σ_0 causes an additional voltage V_0 to be induced across σ_0,

$$V_0 = V_m(\sigma_m - \sigma_0)/[\sigma_0 + (\tfrac{1}{2}z - 1)\sigma_m], \tag{6}$$

where V_m is the voltage drop between adjacent rows far from σ_0, and z, the number of bonds at each node of the network, is 6 for the simple cubic lattice and 4 for the square. If the σ_{ij} are

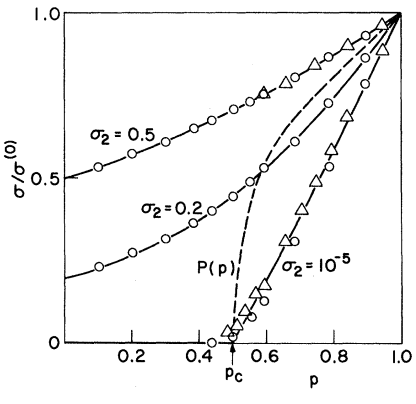

FIG. 2. Conductivity of a two-dimensional square net of conductances with 25×30 nodes, binary disorder. Other labeling conventions as in Fig. 1.

distributed according to some distribution function $p(\sigma)$, the self-consistency condition for σ_m is

$$0 = \langle V_0 \rangle = V_m \int d\sigma\, p(\sigma)(\sigma_m - \sigma)/[\sigma + (\tfrac{1}{2}z - 1)\sigma_m]. \tag{7}$$

The binary distribution, inserted into (7), yields a quadratic equation for σ_m, with the root

$$\sigma_m = \{(\tfrac{1}{2}zp - 1)\sigma_1 + [\tfrac{1}{2}z(1-p) - 1]\sigma_2\}/(z-2) + \left\{\{(\tfrac{1}{2}zp - 1)\sigma_1 + [\tfrac{1}{2}z(1-p) - 1]\sigma_2\}^2 + 2(z-2)\sigma_1\sigma_2\right\}^{1/2}/(z-2), \tag{8}$$

which is plotted as the light solid lines in Figs. 1 and 2. For the cases in which σ_1 and σ_2 are comparable, agreement between (8), appropriately normalized, and the observed conductivities is surprisingly good. For $\sigma_2 \ll \sigma_1$, (8) predicts a linear decrease in σ_m with decreasing p, with σ_m going to σ_2 at $p = \frac{1}{3}$ for the simple cubic net, at $p = \frac{1}{2}$ for the square. The data appear to show this linear dependence in both Figs. 1 and 2, except in the critical regions.

Critical-path analysis.—The effective-medium theory is expected to work best when spatial fluctuations in the current are relatively small. The opposite limit, when most of the current is channeled along the paths of least resistance, occurs at low temperatures, in inelastic hopping conduction among localized states. The localized states may be viewed as the nodes i of a random network of conductances σ_{ij}, with the conductance linking any two states exponentially dependent on the distance between them as well as on their energies.[13] Several authors[4,5] have suggested that at low temperatures the conductivity of such a network, and its temperature dependence, may be estimated by focusing attention on critical paths, and characterizing them by a critical conductance σ_c.

This may be defined by a simple construction, due to Ambegaokar, Halperin, and Langer[4]: The conductances are all removed from the network and replaced one by one, the largest first. The value of σ_{ij} at which extended paths open up is σ_c.

Ambegaokar, Halperin, and Langer argue that for a very broad distribution of σ_{ij}'s, as is obtained at low temperatures, σ may be expressed as $\sigma \approx L^{-1}\sigma_c$, where the prefactor L^{-1} is not determined, but should be less sensitive to the characteristics of the distribution of σ_{ij}'s than is σ_c itself. The temperature dependence of σ is thus taken to be that of σ_c alone, the prefactor adding corrections of order $\ln\sigma_c$ or less. This yields a very simple and elegant derivation of the Mott $T^{-1/4}$ law for conduction at low temperatures.

In an attempt to determine the region of validity of the critical path analysis, we have calculated conductivities of 3D simple cubic networks with the σ_{ij}'s distributed continuously. For a given distribution, both σ_c and, from (7), σ_m are easily obtained.

In case I of Fig. 3, σ_{ij} is distributed uniformly over the interval $(1-A,\ 1+A)$ with the weight factor $p(\sigma) = (2A)^{-1}$. Since $p_c(3D) = 0.25$, $\sigma_c = 1 + \frac{1}{2}A$ and increases, but the network conductivity is observed to decrease, with increasing width of the distribution. As shown in Fig. 3, σ_m gives a close underestimate to σ for all A, the error increasing as A increases. Clearly, for this distribution, conduction is not dominated by the paths of least resistance, and the percolation analysis is irrelevant.

In case II of Fig. 3, a broad distribution more suitable to the critical-path analysis is studied. $\ln\sigma_{ij}$ is distributed uniformly; the σ_{ij}'s range from A^{-1} to A, with $p(\sigma) = (2\sigma \ln A)^{-1}$. For this distribution, σ_m is determined by

$$2\ln A = 3\ln[(A + 2\sigma_m)/A^{-1} + 2\sigma_m)]. \tag{9}$$

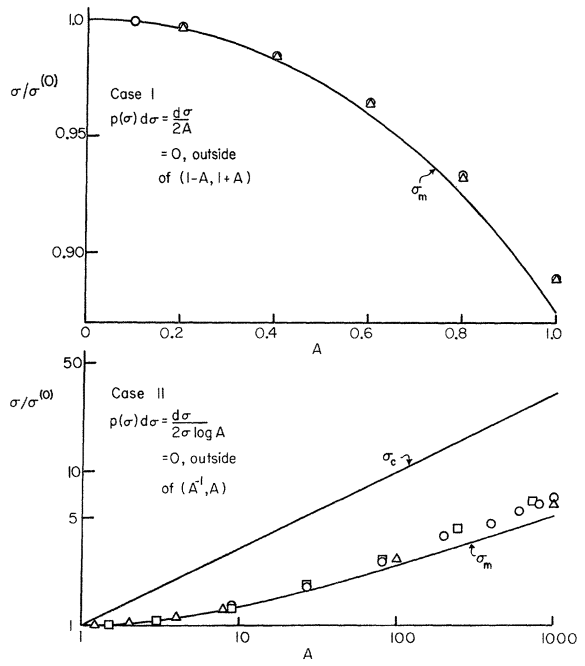

FIG. 3. Conductivity of a simple cubic network of 15^3 nodes, with values of the conductances chosen at random from the distributions $p(\sigma)$ indicated. In the case II plot, both scales are logarithmic, and the critical conductance σ_c has also been plotted.

Solution of (9) for large A yields $\sigma_m = \frac{1}{2}A^{1/3}$, while $\sigma_c = A^{1/2}$. A plot of σ_m, σ_c, and the numerical results for case II, given in Fig. 3, shows that σ_m slightly underestimates the observed conductivity, by a greater amount than in case I. The data points for large A fall roughly on a straight line in this log-log plot, with a slope closer to $\frac{1}{3}$ than to $\frac{1}{2}$.

The logarithmic distribution of case II arises in a description of ionic transport by thermal activation across barriers whose heights are distributed uniformly over a range $\pm \Delta E$ about some average E_0. In this case, we can factor out the average conductance, $\sigma_0(T) \propto \exp(-E_0/kT)$, and identify $\ln A = \Delta E/kT$, $\sigma_m/\sigma_0(T) = \frac{1}{2}\exp(+\Delta E/3kT)$, and $\sigma_c/\sigma_0(T) \propto \exp(+\Delta E/2kT)$ for low T. The effective activation energy $\Delta E/3$, given by the effective-medium theory, is in agreement with the calculated results of Fig. 3, while the prefactor $\frac{1}{2}$ is too low by about 25%. The critical-path analysis gives too large an effective activation energy, and no information about the prefactor. We conclude that the changes with T in the composition of the critical paths and the varying importance of currents along noncritical paths are sufficiently great that $\sigma_c(T)$ alone does not provide a quantitative description of the conductivity, at least for this simple example.

Discussions with D. J. Thouless, Morrel Cohen, and Vinay Ambegaokar are gratefully acknowledged.

*Research supported by the U. S. Army Research Office (Durham) and by the Advanced Research Projects Agency.

†Present address: IBM Research Center, Yorktown Heights, N. Y. 10598.

[1]J. M. Ziman, J. Phys. C: Proc. Phys. Soc., London 1, 1532 (1968); M. H. Cohen, in *Proceedings of the Tenth International Conference on the Physics of Semiconductors, Cambridge, Massachusetts, 1970*, edited by S. P. Keller, J. C. Hensel, and F. Stern, CONF-700801 (U. S. AEC Division of Technical Information, Springfield, Va., 1970), p. 645; R. Zallen and H. Scher, Phys. Rev. B 4, 4471 (1971).

[2]T. P. Eggarter and M. H. Cohen, Phys. Rev. Lett. 25, 807 (1970), and 27, 129 (1971).

[3]N. F. Mott, Advan. Phys. 16, 49 (1967).

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

[5]M. Pollak, to be published.

[6]S. R. Broadbent and J. M. Hammersley, Proc. Cambridge Phil. Soc. 53, 629 (1957); H. L. Frisch and J. M. Hammersley, SIAM (Soc. Ind. Appl. Math.) J. Appl. Math. 11, 894 (1963).

[7]H. L. Frisch, J. M. Hammersley, and D. J. A. Welsh, Phys. Rev. 126, 949 (1962).

[8]V. K. S. Shante and S. Kirkpatrick, Advan. Phys. 20, 325 (1971).

[9]D. A. G. Bruggeman, Ann. Phys. (Leipzig) 24, 636 (1935); R. Landauer, J. Appl. Phys. 23, 779 (1952), and unpublished notes.

[10]B. J. Last and D. J. Thouless, preceding Letter [Phys. Rev. Lett. 27, 1719 (1971)].

[11]H. Fritzsche, in *Electronic Properties of Materials*, edited by R. H. Bube (McGraw-Hill, New York, 1971), Chap. 13.

[12]P. Soven, Phys. Rev. 156, 809 (1967); B. Velický, S. Kirkpatrick, and H. Ehrenreich, Phys. Rev. 175, 747 (1968).

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

[14]N. F. Mott, Phil. Mag. 19, 835 (1969).

Lattice Dynamics of Nb_3Sn-Type Compounds*

L. J. Sham
Department of Physics, University of California, San Diego, La Jolla, California 92037
(Received 28 October 1971)

It is shown that, in the cubic phase, the doubly degenerate Γ_{12} mode is the only long-wavelength optical mode which is temperature dependent in the harmonic approximation. However, it does not become unstable on cooling because it would drive a shear acoustic mode unstable first. The elastic constants are calculated by the method of long waves. Only $C_{11}-C_{12}$ is temperature dependent. Its calculated values for Nb_3Sn are in fair agreement with experiment.

I have developed a method for the first-principles calculation of phonon frequencies in the intermetallic compounds of β-W structure in the harmonic approximation. I have examined the temperature dependence, in the cubic phase, of the long-wavelength optical modes and of the elastic constants, from which can be deduced some knowledge of the existence and the nature of the martensitic transformation in these compounds.

To calculate the electronic polarization which