

Scaling theory of the metal-insulator transition in amorphous materials

W. L. McMillan

Department of Physics and Materials Research Laboratory, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801

(Received 17 July 1980; revised manuscript received 22 December 1980)

A scaling model is presented for the metal-insulator transition in amorphous materials which includes a localization, correlation, and screening. The model predicts a continuous phase transition at zero temperature with localized states and a correlation gap in the insulating phase.

Recent experiments have indicated that the metal-insulator transition in several amorphous or disordered materials [*a*-Ge_{1-x}Au_x,^{1,2} granular alumina,³ and crystalline P-doped Si (Ref. 4)] is continuous. In *a*-Ge_{1-x}Au_x,¹ in particular, measurements of conductivity versus temperature show that the electronic states are extended in the metallic phase and localized in the insulating phase; the transition involves localization and therefore has something of the character of the Anderson transition.⁵ However, tunneling experiments on *a*-Ge_{1-x}Au_x (Ref. 2) and granular alumina³ find a giant zero-bias anomaly in the one-electron density of states of the metal due to electron-electron interaction and also, apparently, a correlation gap in the insulating state. Thus the transition also has something of the character of a Mott transition.⁶

In this paper I develop a scaling theory of the metal-insulator transition in amorphous materials including the effects of localization and correlation. This theory is an extension of the scaling theory of the Anderson transition by Abrahams *et al.*⁵ which treats localization within a one-electron model. Correlation effects are included by adapting a weak-coupling approximation due to Altshuler and Aro-nov⁷ and Altshuler *et al.*⁷ and by screening the electron-electron interaction within linear response theory. The effects of correlation are cast into renormalization-group language using an "exact eigenstates" method.⁸ Included in the theory are one-electron localization, many-body localization, screening, and interaction effects on the one-electron density of states and the correlation gap.

We consider a model for the motion of electron wave packets of length scale L . We assume that the single-particle motion is diffusive with diffusion constant D_L for wave packets of radius L . The wave packets are to be made up of eigenstates $\phi_i(x)$ with eigenvalue $\hbar\omega_i$ of the one-electron problem and chosen to have minimum energy spread F_L . There is a characteristic energy $\hbar D_L/L^2$ associated with D_L which turns out to be the minimum energy spread F_L (within a constant of order unity). We therefore define $F_L = \hbar D_L/L^2$. One can verify this relationship us-

ing the exact eigenstates method⁸ which is discussed below. We write down an unnormalized wave function

$$\psi(x) = \sum_i \phi_i^*(x_0) \phi_i(x) \exp[-\hbar^2(\omega_i - \omega)^2/4F^2]$$

which is centered at x_0 with mean energy $\hbar\omega$ and energy spread F . The mean-square radius is easily found to be

$$\langle (\bar{x} - \bar{x}_0)^2 \rangle = 3\hbar D / \sqrt{2\pi} F$$

in three dimensions. I have also verified this relationship by simulation. This relationship provides a fundamental connection between length scale L and energy scale F_L . We use a renormalization-group approach and adopt a model at length scale L which retains one-electron states within energy F_L of the Fermi energy E_F . Roughly speaking, quantum states ϕ_i with energy $|\hbar\omega_i - E_F| > F_L$ will have been "integrated out" by including their contributions to various physical quantities. More concisely, we will integrate out transitions between quantum state ϕ_i and ϕ_m so that at length scale L transition between states such that $\hbar|\omega_i - \omega_m| > F_L$ have been removed; we actually remove matrix elements from the Hamiltonian, not quantum states. A second physical parameter of the system is the one-electron density of states (of one spin and for a unit volume) N_L at the Fermi energy; we find a second energy scale $E_L = 1/N_L L^3$. We write for the interaction between electrons $U(r) = e^2/\epsilon_L r$, where ϵ_L is the long-wavelength dielectric constant; ϵ_L contains the screening contributions from the quantum states which have been integrated out. The dielectric constant is, of course, a function of wave number q but it is approximately constant for $qL < 1$. The third energy scale is $U_L = e^2/L\epsilon_L$. We believe that the three physical quantities D_L , N_L , and ϵ_L or, equivalently, the three energy scales F_L , E_L , and U_L are sufficient to describe the Hamiltonian of the system at length scale L . We now define two dimensionless parameters from ratios of the energy scales. We first define a conductivity parameter $\sigma_L \equiv 2e^2 N_L d_L$ such that the physical conductivity at zero temperature is $\sigma = \lim_{L \rightarrow \infty} \sigma_L$. Following Abra-

hams *et al.*⁵ we define a dimensionless conductance

$$g_L \equiv 8\sqrt{2}\pi\hbar L \sigma_L / e^2 = 16\sqrt{2}\pi F_L / E_L .$$

The second dimensionless parameter is the dimensionless interaction strength $\lambda_L \equiv 16U_L / E_L$. We derive below the renormalization-group (RG) equations for g_L and λ_L .

We will use the exact eigenstates method⁸ to calculate various physical quantities. We assume a one-electron Hamiltonian with eigenstates $\phi_l(x)$ normalized in unit volume and eigenvalues $\hbar\omega_l$. We require certain averages of the matrix element

$$M_{lm}(q) \equiv \int d^3x \phi_l^*(x) e^{-i\vec{q}\cdot\vec{x}} \phi_m(x) . \quad (1)$$

which we derive as follows. We make up a wave packet

$$\psi(x,t) = \sum_l \phi_l^*(x_0) \phi_l(x) \frac{e^{-i\omega_l t}}{\sqrt{n}} \quad (2)$$

from n quantum states and assume diffusive motion of the wave packet

$$|\psi(x,t)|^2 = \frac{\exp[-(x-x_0)^2/4Dt]}{(4\pi Dt)^{3/2}} . \quad (3)$$

Fourier-transforming both sides of Eq. (3) in space $\int d^3x e^{-i\vec{q}\cdot(\vec{x}-\vec{x}_0)}$ and time $\int_0^\infty dt e^{i\omega t - \eta t}$, space averaging $\int d^3x_0$, and taking the imaginary part we find the average of the matrix element squared over all states with fixed energy difference $\hbar(\omega_l - \omega_m)$ (Ref. 7)

$$|M_{lm}(q)|^2 = (Dq^2/\pi N_L \hbar) / [(\omega_l - \omega_m)^2 + D^2 q^4] . \quad (4)$$

We now change length scale from L to L' by changing the energy cutoff from $F_L = \hbar D_L / L^2$ to $F_{L'} = \hbar D_{L'} / L'^2$; to lowest order in λ and g^{-1} , D_L is independent of L and $d \ln F / d \ln L = -2$. We change energy scale from F_L to $F_{L'}$ by including the contribution to all physical quantities from transitions between states l and m such that $F_{L'} < \hbar|\omega_l - \omega_m| < F_L$. The contribution to the long-wavelength dielectric constant is

$$d\epsilon = \lim_{q \rightarrow 0} \frac{16\pi e^2}{q^2} \sum_{lm} |M_{lm}(q)|^2 \frac{f_l(1-f_m)}{\hbar(\omega_m - \omega_l)} , \quad (5)$$

where f_l is the occupation number of the l th state and the summation is over all states such that $F_{L'} < \hbar|\omega_l - \omega_m| < F_L$. Performing the integrals we find

$$\frac{d \ln \epsilon_L}{d \ln L} = +2\lambda_L . \quad (6)$$

We next calculate the renormalization of the density of states which is given by $(1 + d\Sigma_m/d\hbar\omega_m)^{-1}$ where Σ_m is the self-energy of the m th state. We use the

Hartree-Fock approximation. The Hartree term screens the one-electron potential and the contribution from the exchange term is

$$d \left(1 + \frac{d\Sigma_m}{d\hbar\omega_m} \right) = - \sum_l \sum_q U_q \frac{d}{d\hbar\omega_m} |M_{lm}(q)|^2 f_l , \quad (7)$$

where the sum is restricted by $F_{L'} < \hbar|\omega_l - \omega_m| < F_L$ and $U_q = 4\pi e^2/q^2 \epsilon_L$ is the Fourier transform of the interaction. Performing the integrals we find

$$\frac{d \ln N_L}{d \ln L} = - \frac{\lambda_L}{g_L} . \quad (8)$$

Finally we need to calculate the renormalization of the diffusion constant. Instead of developing the exact eigenstates formalism to calculate the conductivity we will adapt the perturbative calculation of Altshuler and Aronov⁷ to our purposes. These authors find for the renormalization of the zero frequency, zero-temperature conductivity

$$\frac{d\sigma}{\sigma} = \frac{4\pi}{3} \int_{F_{L'}}^{F_L} E dE \sum_q U_q \text{Re}(iE + D_q^2)^{-3} . \quad (9)$$

The perturbative calculation yielded limits on the energy integral from zero to infinity and we have modified that result by summing only over transitions between $F_{L'}$ and F_L . Carrying out the integrals we find

$$\frac{d \ln \sigma_L}{d \ln L} = - \frac{2\lambda_L}{g_L} . \quad (10)$$

From the definition of σ_L we have

$$\frac{d \ln D_L}{d \ln L} = \frac{d \ln \sigma_L}{d \ln L} - \frac{d \ln N_L}{d \ln L} \quad (11)$$

so that Eqs. (8), (10), and (11) determine the renormalization of the diffusion constant due to interactions. There is also a one-electron contribution to the renormalization of the diffusion constant which, according to Abrahams *et al.*,⁵ is of the form $-c/g_L$ with c unknown. The above results are valid within perturbation theory, $\lambda_L \ll 1$, $1/g_L \ll 1$.

Assembling these results we find

$$\begin{aligned} \frac{d \ln N}{d \ln L} &= - \frac{\lambda}{g} , & \frac{d \ln \epsilon}{d \ln L} &= 2\lambda , \\ \frac{d \ln D}{d \ln L} &= - \frac{(c+\lambda)}{g} , & \frac{d \ln E}{d \ln L} &= -3 + \frac{\lambda}{g} , \\ \frac{d \ln F}{d \ln L} &= -2 - \frac{(c+\lambda)}{g} , & \frac{d \ln U}{d \ln L} &= -1 - 2\lambda , \\ \frac{d \ln g}{d \ln L} &= 1 - \frac{(c+2\lambda)}{g} , \\ \frac{d \ln \lambda}{d \ln L} &= 2 - 2\lambda - \frac{\lambda}{g} . \end{aligned} \quad (12)$$

Equations (12) are the differential equations of the

two-parameter renormalization group, derived within weak coupling ($\lambda \ll 1$, $g^{-1} \ll 1$). The first correction term in the conductance equation is the one-electron localization correction of Abrahams *et al.*⁵; we interpret the second term as a many-body localization correction. We feel comfortable extrapolating the RG equations to intermediate coupling to study the phase transition.

We now study the properties of the RG equations. We first study the RG trajectories in parameter space to locate the fixed points representing phase transitions and stable phases. The constant c is unknown; however, we expect the qualitative behavior of the theory to be insensitive to the value of the constant. We will work through the theory with the value $c = \frac{7}{4}$, chosen so that one-particle localization and many-body localization are of equal importance at the phase transition. With this value of c the flow diagram is given in Fig. 1. There is a fixed point at $(g, \lambda) = (\frac{7}{4}, 0)$ which represents the Anderson transition studied by Abrahams *et al.*⁵ The trajectory to the right is toward $(\infty, 0)$ which represents the noninteracting conducting state with extended states; the trajectory to the left is toward $(0, 0)$ which represents the noninteracting insulating state with localized quantum states. The Anderson-transition fixed point is unstable with respect to interactions and does not represent an observable metal-insulator transition (according to the present theory) although it can represent a mobility edge far from the Fermi energy. The noninteracting insulator and conducting states are not physically observable states. The fixed point at $(\frac{7}{2}, \frac{7}{8})$ represents the metal-insulator transi-

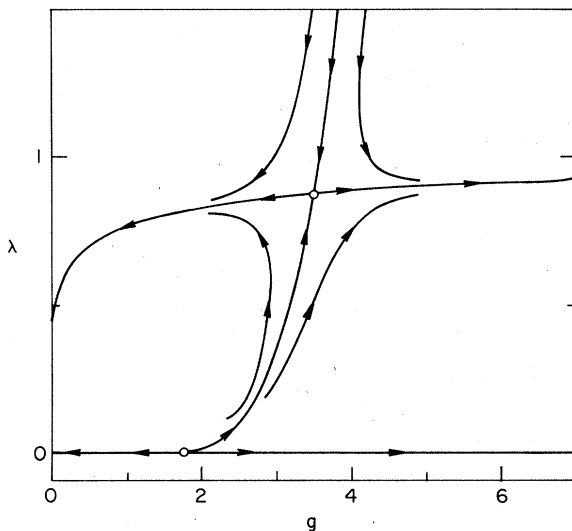


FIG. 1. Flow diagram of the two-parameter renormalization group showing trajectories in parameter space with the two fixed points marked by open circles.

tion in the interacting system and the two trajectories flowing into it are the critical surface separating parameter space into two regions, conducting on the right and insulating on the left. On the right the flow is toward $(\infty, 1)$ which represents an observable phase which we call the amorphous conductor phase. On the left the flow approaches the λ axis as g goes to zero which represents an observable phase which we call the amorphous insulator phase. We show below that these two phases have unique, universal properties which depend only on a length scale ξ and an energy scale Δ .

We now study the fixed point at $(\frac{7}{2}, \frac{7}{8})$ and develop the scaling theory. We start the calculation at microscopic length scale " a " with properties N_a , etc. If we start on the critical surface we find $E_L = E_a(a/L)^\eta$, $F_L = F_a(a/L)^\eta$, $U_L = U_a(a/L)^\eta$, $D_L = D_a(a/L)^{\eta-2}$, $\epsilon_L = \epsilon_a(a/L)^{1-\eta}$, $N_L = N_a(a/L)^{3-\eta}$, $\sigma_L = \sigma_a(a/L)$, with $\eta = \frac{11}{4}$. We now linearize the differential equations near the fixed point and find a single positive eigenvalue of $\sqrt{17/8} - \frac{1}{2} = 0.96$. Making the usual renormalization-group arguments⁹ the correlation length ξ (at which the system crosses over from the critical regime to the conducting or insulating regime) is proportional to $|x - x_c|^{-\nu}$ where $\nu^{-1} = 0.96$ and x is the composition with x_c the critical composition. We assume here that composition is the external control parameter that drives the system through the transition (at zero temperature). Thus we find two critical exponents η , relating energy scale and length scale in the critical regime, and ν , relating correlation length and composition. Both exponents depend upon the value of the constant c and upon the way in which the theory is extrapolated from weak coupling and therefore the numerical values should not be taken seriously. We have $1 < \eta < 3$ and we expect $\nu \approx 1$. The energy scale of the system as it crosses over from the critical regime to the conducting or insulating regime is

$$\Delta \equiv F_\xi = \hbar D_\xi / \xi^2 = (\hbar D_a / a^2) (a/\xi)^\eta.$$

We now discuss the properties of the system in the three regimes: critical, conducting, and insulating. In what follows we will estimate the order of magnitude of various quantities and will omit constants of order unity. In order to estimate properties of the system at finite energy E , frequency ω , or temperature T , we stop the renormalization group at a length scale such that the energy scale is E or $\hbar\omega$ or kT . In the critical regime at finite temperature we stop at a length scale $L_T = a (F_a/kT)^{1/\eta}$ and find for the conductivity

$$\sigma(T) = \sigma_a(a/L_T) = \sigma_a(kT/F_a)^{1/\eta}.$$

Similarly at finite frequency $\sigma(\omega) = \sigma_a(\hbar\omega/F_a)^{1/\eta}$. The one-electron density of states versus energy is

$N(E) = N_a(E/F_a)^{-1+3/\eta}$. The Coulomb interaction is partially screened $U(r) = (e^2/\epsilon_a)(a/r)^\eta$. In the conducting regime the solution to the RG equations are $\lambda = 1$, $g_L = 3.5(1 + L/\xi)$. We find

$$\sigma_L = 0.1(e^2/\hbar\xi)(1 + \xi/L)$$

and energy scale $F_L = \Delta(\xi/L)^2$. The length scale at finite temperature is $L_T = \xi\sqrt{\Delta/kT}$ and the conductivity at finite temperature is therefore

$$\sigma(T) = 0.1(e^2/\hbar\xi)(1 + \sqrt{kT/\Delta})$$

Solving the differential equation for the density of states we find $N_L = N_\xi(1 + \xi/L)/2$ so that the density of states versus energy is

$$N(E) = N_a(a/\xi)^{3-\eta}(1 + \sqrt{E/\Delta})$$

The dielectric constant is

$$\epsilon_L = \epsilon_a(\xi/a)^{\eta-1}(L/\xi)^2$$

and

$$\epsilon_q = \epsilon_a(\xi/a)^{\eta-1}/(q\xi)^2 ;$$

this implies exponential screening with a screening length ξ . The theory behaves sensibly in the insulating regime. The conductance goes to zero at a finite length scale ξ which we interpret as the localization length. The dielectric constant goes to a constant $\epsilon = (\epsilon_a)(\xi/a)^{\eta-1}$ and the Coulomb energy $U_\xi = \Delta = U_a(a/\xi)^\eta$, which is the relevant energy scale in the insulating phase, is finite. The density of states goes sharply to zero and there is a correlation energy gap equal to Δ . The conductivity goes quickly (exponentially) to zero for $kT < \Delta$. All these properties are undoubtedly characteristic of the amorphous insulating phase. We do not, of course, expect a sharp energy gap in the density of states; we expect band tailing below Δ . At present we have no viable microscopic model of the amorphous insulating phase; the theory presented above in deriving the RG equations is a primitive microscopic theory of the amorphous conducting phase.

There is a characteristic conductivity which separates normal metallic behavior from the amorphous conductor behavior. In the normal metallic regime the conductivity is $e^2k_F^2l/3\pi^2\hbar$, where k_F is the Fermi wave number and l the mean free path; this description breaks down for mean free path less than atomic spacing "a" (we assume a macroscopically homogeneous material). Since $k_F a$ is a typically π , the normal-metal regime is for $\sigma > e^2/3\hbar a$. The conductivity in the amorphous conducting regime is $0.1e^2/\hbar\xi$ which should apply when $\xi > a$ or $\sigma < 0.1e^2/\hbar a$. Therefore we expect a crossover from normal metallic behavior, with σ decreasing with increasing temperature, to amorphous metallic behavior, with σ increasing with increasing temperature for $\sigma \approx 0.2e^2/\hbar a$ which is a resistivity of about

200 $\mu\Omega$ cm for metals.

The theory predicts a strong universality: all metal-insulator transitions in (macroscopically homogeneous) disordered materials should have the same exponents. Further, since the only relevant parameters are the length scale ξ and energy scale Δ , both the amorphous insulator and amorphous conductor phases should obey a law of corresponding states. The materials must be homogeneous on a length scale larger than ξ to avoid the complication of a classical percolation problem. I see no reason why the theory should not be applicable to granular materials provided the correlation length is larger than the grain size and the material is homogeneous; presumably, the critical region will be narrower for granular materials.

It is clearly desirable to have a more detailed picture of the conducting and insulating phases than that presented here. One wants to use the renormalization-group approach for $L < \xi$ to find the Hamiltonian parameters for $L = \xi$ and then develop a microscopic theory using the Hamiltonian. The physical picture of the conducting phase is pretty clear. There is electron-hole symmetry (in both phases). There is a square-root anomaly in the one-electron density of states which is a precursor to the opening of the correlation gap at the transition. The screening length is ξ and the electron-electron interaction is strong and is the dominant interaction. A somewhat more sophisticated calculation of the self-energy using the screened exchange approximation shows that the quasiparticle approximation is valid for energies much less than Δ but breaks down for $E \approx \Delta$ due to electron-electron scattering. The conductivity mechanism at low temperatures is quantum diffusion of quasiparticles; the quantum states are, or course, extended in the Anderson sense. Since the density-of-states renormalization for each spin direction follows the Fermi energy for that spin, the spin susceptibility is not renormalized. In the insulating phase it is clear that there is a correlation gap but there is, at present, no satisfactory microscopic model of that phase.

The present experimental situation is as follows. The metal-insulator transition appears to be continuous in a -Ge_{1-x}Au_x,¹ granular alumina,³ and, possibly, phosphorus-doped silicon.⁴ Certainly one can make samples with very small conductivities; it is not clear at what point inhomogeneities and classical percolation become important. The observation of correlation effects by tunneling experiments² in a -Ge_{1-x}Au_x motivated the present theoretical work. More recent tunneling experiments on granular alumina³ have shown that the square-root anomaly in the density of states scales with the conductivity over several decades and that $\eta \approx 2$; this is the first real test of the scaling theory. Tunneling experiments² in the insulating phase indicate an absence of available

states at low energy and thus an energy gap; however, a quantitative interpretation of the experiment requires an understanding of field penetration into the insulator which requires a detailed model of the insulating phase. The conductivity crosses over from an exponential dependence (with a fractional inverse power of T) at low temperature to an algebraic dependence at high temperature. The crossover temperature is a characteristic energy which might be interpreted as an energy gap; however, one could alternatively interpret this behavior as a crossover from variable-ranged hopping⁶ at low temperature to nearest-neighbor hopping at high temperature. Thus, the experimental evidence for an energy gap is ambiguous. In summary, the experimental evidence is

strong that correlation and localization effects are important near the metal-insulator transition and one scaling prediction has been tested experimentally. However, many of the predictions of the theory await experimental confirmation.

ACKNOWLEDGMENTS

The author would like to thank B. Dodson, R. C. Dynes, and J. Mochel for extensive discussions of their experiments and P. W. Anderson and P. A. Lee for theoretical discussions. I would also like to acknowledge support by the National Science Foundation under Grant No. NSF-DMR-77-27091.

¹B. M. Dodson, W. L. McMillan, J. M. Mochel, and R. C. Dynes, Phys. Rev. Lett. 46, 46 (1981).

²W. L. McMillan and J. Mochel, Phys. Rev. Lett. 46, 556 (1981).

³R. C. Dynes and J. Garno, Phys. Rev. Lett. 46, 137 (1981).

⁴T. F. Rosenbaum, K. Andres, G. A. Thomas, and R. N. Bhatt, Phys. Rev. Lett. 45, 1723 (1980).

⁵E. Abrahams, P. W. Anderson, D. C. Licciardello, and T. V. Ramakrishnan, Phys. Rev. Lett. 42, 673 (1979).

⁶N. F. Mott, *Metal-Insulator Transitions* (Taylor and Francis, London, 1974).

⁷B. L. Altshuler and A. G. Aronov, Zh. Eksp. Teor. Fiz. 77, 2028 (1979) [Sov. Phys. JETP 50, 968 (1979)]; B. L. Altshuler, A. G. Aronov, and P. A. Lee, Phys. Rev. Lett. 44, 1288 (1980).

⁸E. Abrahams, P. W. Anderson, P. A. Lee, and T. V. Ramakrishnan (unpublished).

⁹K. Wilson and J. Kogut, Phys. Rep. C 12, 75 (1974).