Dephasing and Anderson localization in topologically disordered systems

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A simple theory is developed to describe the interplay between Anderson localization and dephasing mechanisms (such as inelastic electron- or exciton-phonon coupling), within the framework of a tight-binding model of spatially disordered systems. Self-consistency is enforced by demanding that only the most probable value of the imaginary part of the site self-energy be self-consistently determined. Dephasing interactions are characterized simply by an energy-independent dephasing rate. When the dephasing rate vanishes the pure localization problem may be examined as the transition is approached from either the localized or the extended regimes; mobility-edge trajectories may thereby be located. In the limit of rapid dephasing the theory correlates with the usual master-equation treatments of incoherent transport. For sufficiently large disorder a nonmonotonic but continuous crossover from coherent to incoherent transport is in general predicted. The problem of Mooij correlation, viewed as a weak-delocalization phenomenon, is also examined: it is suggested that the correlation is not universal as has frequently been supposed.

I. INTRODUCTION

The localization phenomenon discovered by Anderson¹ is both the simplest and most subtle concept in the theory of quantum transport. It is simple because its physical content arises directly from the description of single particle transport in terms of probability amplitudes and the superposition principle. Its inherently quantum nature also makes localization subtle. Interactions which destroy phase relationships can act to mask the Anderson localization: such dephasing effects lead to the phenomena of self-trapping and incoherent hopping transport which are manifest in many experiments. Also, because these phenomena can be visualized in a nearly classical way, there has been an occasional tendency to confuse them with Anderson localization itself, especially when the localization idea is used in the context of topologically disordered materials such as electrons in fluids and exciton transport in disordered solids.

The importance of the interplay between dephasing and Anderson localization has been realized by many workers (for recent reviews see Refs. 2–5). In the area of weak delocalization in dirty metals, the effects of inelastic scattering which give rise to dephasing, and of magnetic fields which modify phase relationships, have been paramount in elucidating the scaling theory of localization.^{2–5,6,7} In this paper we would like to take a different direction by pointing out how dephasing enters into a mean-field theory of localization in topologically disordered systems. In so doing we present an approximate but unified picture of the coherent quantum transport considered in the localization theory, and the incoherent transport usually considered in these systems.

The theory we develop has its origins in the treatment

of localization on a Cayley tree due to Abou-Chacra, Anderson, and Thouless^{8,9} (AAT). In previous papers^{10–12} we have shown how their treatment can be extended to include the effects of short-range structure and of band structure in spatially disordered materials. These theories start with the locator expansion and use the notion that there is a site self-energy which is a random variable whose probability distribution can be self-consistently determined. Rather than solving completely the resultant nonlinear integral equations, however, the theories ultimately reduce to a stability analysis of the localized states. They do not therefore yield direct estimates for the rate of transport, although they do reasonably well at locating mobility edges, especially when band-structure effects are taken into account.¹²

A generalization of the nonlinear integral equations to include dephasing is straightforward. With dephasing, however, something more than a stability analysis is required. This step was taken for the Cayley-tree problem by Jonson and Girvin.^{13,14} In attractive pioneering papers they analyzed the problem via a Monte Carlo procedure. Although their analysis led to many interesting ideas, we feel that the Monte Carlo procedure also led to some misleading conclusions. In particular, the available and possibly inadequate statistics led Girvin and Jonson to support the idea of a discontinuous localization transition. The existence of a minimum metallic conductivity would contradict the emerging scaling ideas for finitedimensional systems, 2^{-5} although the status of discontinuous localization on a Cayley tree is still controversial: recent results based on supersymmetric field-theory treatments have come to various conclusions.^{15–17}

In this paper we simplify the self-consistency conditions in such a way that we have to analyze algebraic equations rather than integral equations, by demanding that only the most probable value of the imaginary part of the site self-energy be self-consistently determined. The increased transparency introduced by this simplification allows a rather complete analysis, and the simplified self-consistent theory exhibits many healthy features. When the dephasing rate vanishes the pure localization problem may be examined as the transition is approached from either the localized regime or the domain of extended states. The theory locates mobility edges rather well, and provides a reasonable estimate for the Anderson transition density. The simplified treatment predicts a continuous transition, with which we believe an exact analysis of the full integral equations would concur; critical exponents for the electrical conductivity may also be deduced. In the limit of large dephasing the theory here developed correlates with the usual master-equation treatments of incoherent transport, and a nonmonotonic but continuous crossover from coherent to incoherent transport is predicted. The problem of Mooij correlation¹⁸ found for electron transport in dirty metals, viewed as a weak-delocalization phenomenon, may also be addressed within the present theory. Results compatible with experimental observation are obtained and, in agreement with the recent work of Tsuei,¹⁹ it is found that the correlation is not universal as has frequently been supposed.

In Sec. II A we derive the self-consistency equations basic to the present theory, in which the effects of dephasing are included. Central to our discussion is the random multicomponent reference system introduced by us previously.^{10,11} This consists of atoms or molecules, each possessing a random self-energy and mutually interacting via an appropriately chosen classical interaction potential (which for convenience is assumed spherically symmetric and pairwise additive). In Sec. IIB we examine the asymptotic behavior of the distribution function $f(\Delta)$ for the imaginary part $-\Delta$ of the site self-energy. A knowledge of the asymptotic properties of $f(\Delta)$ enables us to construct an explicit self-consistent algebraic equation for the most probable value, Δ_m , of Δ . The pure localization problem is examined in Sec. III A by analysis of the self-consistency equation for Δ_m appropriate to a vanishing dephasing rate. Critical exponents for the transition are determined, an explicit expression is deduced for Δ_m in the domain of extended states, and the general results are illustrated by application to a specific problem. The effects of a nonzero dephasing rate, and the interplay between localization and dephasing, are investigated in Sec. III B; a rich variety of physical behavior is found, as alluded to above. Finally, in Sec. III C the problem of Mooij correlation¹⁸ is examined within the framework of the present theory.

II. THEORY

A. Derivation of the basic equations

In previous work $^{10-12}$ we have developed a selfconsistent theory of localization in a tight-binding model of spatially disordered systems, a central element of which is the disordered reference system mentioned in Sec. I. Following AAT,⁸ this approach to localization centers on a probabilistic analysis of the following equation for the self-energy obtained from second-order renormalized perturbation theory²⁰ (which is exact for a Cayley tree):

$$S_{i}(Z) = \sum_{j(\neq i)} \frac{|V_{ij}|^{2}}{Z - \varepsilon_{j} - S_{j}(Z)} = E_{i}(Z) - i\Delta_{i}(Z) . \qquad (2.1)$$

Here $\{\varepsilon_i\}$ are the site energies and $\{V_{ij}\}$ the transfermatrix elements. The former are assumed to be independent random variables with a given distribution $P(\varepsilon_i)$; the source of off-diagonal disorder (randomness in the V_{ij} 's) is taken to be the topological disorder inherent in the Boltzmann center-of-mass distribution for particles interacting via the chosen classical potential. $Z = E + i\eta$ where *E* is the energy and η a positive infinitesimal. With (2.1) the question of whether or not states of energy *E* are localized becomes one of self-consistency, by demanding that the probability distributions of the self-energies on either side of (2.1) be self-consistently determined.

In the usual approach to localization, one starts from the assumption that states of energy E are localized $[\Delta_i(E) \propto \eta]$, so that (2.1) reduces to

$$E_i \simeq \sum_j' \frac{|V_{ij}|^2}{E - \varepsilon_j - E_j} ,$$

$$\Delta_i \simeq \sum_j' \frac{|V_{ij}|^2 (\eta + \Delta_j)}{(E - \varepsilon_j - E_j)^2} .$$
(2.2)

By employing (2.2), and averaging over the disordered reference system, a nonlinear integral equation is derived¹¹ for the joint probability distribution function $F(E_i, \Delta_i)$. The limits of stability of localized states with energy E are inferred from the limits of stability of solutions to the derived integral equation: When a solution exists the states are localized, and when there is no solution states are assumed to be extended.

With the above procedure, one can study the breakdown of localized states with decreasing disorder (such as increasing density); in particular, one locates mobilityedge trajectories reasonably well. Unfortunately, however, and by virtue of the assumption leading to (2.2), one cannot work from the other extreme to study how extended states collapse with increasing disorder to form localized states. To do this necessitates consideration of the full equations obtained from (2.1) for the real and imaginary parts of S_i , which are given by

$$E_{i} = \sum_{j}' \frac{|V_{ij}|^{2} (E - \varepsilon_{j} - E_{j})}{(E - \varepsilon_{j} - E_{j})^{2} + (\eta + \Delta_{j})^{2}} , \qquad (2.3a)$$

$$\Delta_{i} = \sum_{j}' \frac{|V_{ij}|^{2} (\eta + \Delta_{j})}{(E - \varepsilon_{j} - E_{j})^{2} + (\eta + \Delta_{j})^{2}} .$$
(2.3b)

By averaging over the disordered reference system a general nonlinear integral equation may be derived for $F(E_i, \Delta_i)$, which in its full form is hopelessly intractable.^{8,21} One aim of this paper is to analyze this problem in an approximate but physically transparent manner by enforcing self-consistency not on the full probability distribution function, but on the most probable value of the imaginary part of the self-energy.

As mentioned in Sec. I, a second aim of the paper is to incorporate the effects of dephasing, and to examine the interplay between dephasing and Anderson localization. When analyzing the zero-temperature localization problem by itself, the imaginary part of the energy, η , is taken as infinitesimally small. As pointed out by Thouless and Kirkpatrick,²² however, retention of finite η is equivalent to introducing a dephasing process characterized by a time scale $\tau = \hbar/2\eta$. The specific physical source of dephasing depends of course on the problem under investigation. With low-temperature electronic transport in dirty metals for example, a nonzero η (corresponding to the imaginary part of the dynamical electron-phonon selfenergy¹⁴) simulates the effects of inelastic scattering caused by electron-phonon interactions (although strictly speaking the assumption of a Poissonian process for the scattering is only realistic for white-noise phonons). When considering the transport of electronic excitons, τ might correspond to a lifetime for excitation decay at a given site, caused for example by fluorescence or additional nonradiative processes; and in dealing with vibrational excitons in liquids, τ might represent a time scale characterizing pure dephasing processes.

In this paper then, η is to be regarded as a parameter characterizing the time scale of dephasing interactions. To derive our basic self-consistency equations we define the averaged distribution $f(\Delta_i)$ by

$$f(\Delta_i) = \int_{-\infty}^{+\infty} dE_i F(E_i, \Delta_i) .$$
(2.4)

The most probable value of $f(\Delta_i)$ (for a given energy *E*) will be denoted by Δ_m . We now consider a specific particle, *i*, immersed in the random multicomponent reference system such that the imaginary parts of the self-energies of all particles $j \neq i$ are constrained to have the value Δ_m . E_i and Δ_i are thus given by

$$E_i = \sum_{j}' \frac{|V_{ij}|^2 (E - \varepsilon_j - E_j)}{(E - \varepsilon_j - E_j)^2 + \mu^2} \equiv \sum_{j}' |V_{ij}|^2 X_j , \qquad (2.5a)$$

$$\Delta_{i} = \sum_{j}' \frac{|V_{ij}|^{2} \mu}{(E - \varepsilon_{j} - E_{j})^{2} + \mu^{2}} \equiv \sum_{j}' |V_{ij}|^{2} Y_{j} .$$
(2.5b)

where $\mu = \eta + \Delta_m$. By averaging over the multicomponent reference system, an explicit functional form for

 $f(\Delta_i)$ is determined as a function of Δ_i and μ . Selfconsistency is enforced by requiring that the most probable value of the resultant distribution $f(\Delta_i)$ be equal to the ("input") most probable value, Δ_m .

With this procedure, $F(E_i, \Delta_i)$ is given by

$$F(E_i, \Delta_i) = \left\langle \int \cdots \int \prod_j' dE_j d\Delta_j d\varepsilon_j P(\varepsilon_j) F(E_j, \Delta_j) \right.$$
$$\times \delta \left[E_i - \sum_j' |V_{ij}|^2 X_j \right]$$
$$\times \delta \left[\Delta_i - \sum_j' |V_{ij}|^2 Y_j \right] \right\rangle_{\Gamma},$$
(2.6a)

where the angular brackets denote an average over the phase space Γ of particles interacting via the chosen classical interaction potential. Thus

$$f(\Delta_i) = \left\langle \int \cdots \int \prod_j' dE_j d\varepsilon_j P(\varepsilon_j) f_0(E_j) \right. \\ \times \delta \left[\Delta_i - \sum_j' |V_{ij}|^2 Y_j \right] \right\rangle_{\Gamma},$$
(2.6b)

where

$$f_0(E_j) = \int_{-\infty}^{+\infty} d\Delta_j F(E_j, \Delta_j)$$
(2.6c)

(for any j). From (2.6a), the function f_0 is given by solution of the following integral equation:

$$f_{0}(E_{i}) = \left\langle \int \cdots \int \prod_{j}' dE_{j} d\varepsilon_{j} P(\varepsilon_{j}) f_{0}(E_{j}) \right.$$
$$\times \delta \left[E_{i} - \sum_{j}' |V_{ij}|^{2} X_{j} \right] \right\rangle_{\Gamma} .$$
(2.6d)

With f_0 known, Eq. (2.6b) constitutes an explicit form for $f(\Delta_i)$; self-consistency is then enforced in the manner referred to above.

To reduce (2.6b) and (2.6d) to a usable form, we define the Fourier transform

$$\hat{f}(k) = \int_{-\infty}^{+\infty} d\Delta_i \exp(ik\Delta_i) f(\Delta_i) , \qquad (2.7)$$

and similarly for $\hat{f}_0(k)$. From (2.6b) $\hat{f}(k)$ is given by

$$\widehat{f}(k) = \left\langle \left\langle \exp\left[ik \sum_{j}^{\prime} \left[\frac{|V_{ij}|^2 \mu}{(E - \varepsilon_j - E_j)^2 + \mu^2} \right] \right] \right\rangle \right\rangle \Gamma_{\{E_j, \varepsilon_j\}}$$
(2.8a)

where the double angular brackets denote an average over the reference system. Equation (2.8a) is formally equivalent to 10,11,23

$$\widehat{f}(k) = \exp(-\Delta\mu_{\rm int}/k_B T) , \qquad (2.8b)$$

where T is the temperature; $\Delta \mu_{int}$ is the excess interaction chemical potential for atom *i* dissolved in the multicomponent reference fluid when it interacts with the other atoms in the system via the complex "potential" U(i,j), embodied in the argument of the exponential in (2.8a). As discussed elsewhere,¹¹ $\Delta \mu_{int}$ may be calculated by the standard Onsager-Kirkwood charging strategy of liquid-state theory; for convenience we assume $V_{ij} = V(|\mathbf{R}_i - \mathbf{R}_j|)$ (where \mathbf{R}_i denotes the center of mass of particle *i*). With this procedure, discussed in detail in Ref. 11, Eq. (2.8a) reduces to

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$$\hat{f}(k) = \exp\left\{4\pi\rho \int_{0}^{\infty} dR \ R^{2}g_{0}(R) \int_{-\infty}^{+\infty} dZ \ M(Z) \left[\exp\left(\frac{ik |V(R)|^{2}\mu}{Z^{2} + \mu^{2}}\right) - 1\right]\right\},$$
(2.9a)

where

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$$M(Z) = \int_{-\infty}^{\infty} d\varepsilon f_0(E + Z - \varepsilon) P(\varepsilon) .$$
(2.9b)

 ρ is the number density of particles and $g_0(R)$ the pair distribution function for particles interacting via the chosen classical interaction potential $U_0(R)$. We note in passing that the reduction from (2.8a) to (2.9a) is exact for a perfectly random, spatially uncorrelated system.

A similar analysis, starting from (2.6d) and employing the charging strategy, may also be applied to derive the integral equation satisfied by $\hat{f}_0(k)$; specific details are given in Ref. 11. The resultant integral equation is given by

$$\hat{f}_{0}(k) = \exp\left\{-4\pi\rho \int_{0}^{\infty} dR \ R^{2}g_{0}(R) \left[1 - \int_{-\infty}^{\infty} \frac{dk'}{2\pi} \int_{-\infty}^{\infty} dZ \ \hat{P}(k')\hat{f}_{0}(k') \times \exp\left[-ik'(E-Z) + \frac{ik \|V(R)\|^{2}Z}{Z^{2} + \mu^{2}}\right]\right]\right\}, \quad (2.10)$$

where $\hat{P}(k)$ is the Fourier transform of $P(\varepsilon)$. An approximate solution to this equation in the $\mu \rightarrow 0$ limit, and with $P(\varepsilon)$ given by a Lorentzian distribution, is described in Ref. 11.

Equation (2.9) is the central equation of this section and the starting point for our analysis. With f_0 given by solution of (2.10), and a given functional form for $P(\varepsilon)$, M(Z)in (2.9b) is known explicitly. Equation (2.9a) then constitutes an explicit expression for $\hat{f}(k)$ and thus $f(\Delta)$. Selfconsistency is enforced by requiring that the most probable value of the resultant distribution $f(\Delta)$ be equal to the most probable value Δ_m (= $\mu - \eta$) in Eqs. (2.5); this leads to a self-consistent algebraic or transcendental equation to be solved for Δ_m . The pure localization problem corresponds to the $\eta \rightarrow 0+$ limit of the resultant selfconsistency equation. When in this limit the solution for Δ_m is found to be finite, states at the given energy are extended at the density under consideration; in contrast, if Δ_m is found to be proportional to η , states at the given energy are localized. Mobility edges are located by searching for that value of ρ (or appropriate parameters specifying the disorder) at which a transition between the two regimes occurs. The method developed here is thus capable of bridging the domains of localized and extended states by examining either the breakdown of localized states with decreasing disorder, or the collapse of extended states with increasing disorder. In addition, the method enables us to assess the interplay between localization and dephasing by examining the self-consistency problem as a function of the dephasing time scale $\tau = \hbar/2\eta$.

The derivation of (2.9) outlined above stems from the approximate but physically transparent starting equations, (2.5). We note, however, that (2.9) may also be derived via a systematic reduction of the full equation for $F(E_i, \Delta_i)$ obtained from Eq. (2.3).

In the following section we consider the asymptotic behavior of $\hat{f}(k)$ and $f(\Delta)$ in the large- and small- μ limits.

B. Asymptotic behavior of $f(\Delta)$

We consider first the behavior of $f(\Delta)$ in the $\mu \rightarrow 0+$ limit, i.e., the limit in which $\eta \rightarrow 0+$ and $\Delta_m \propto \eta$, corresponding to the regime of localized states in the absence of dephasing interactions.

In this limit the Z = 0 value of the function M(Z), Eq. (2.9b), is directly related to the system's density of states defined by $D(E) = -\pi^{-1} \langle \langle \operatorname{Im} G_{ii}^{(+)}(E) \rangle \rangle$, where $G_{ii}^{(+)}(E) = \lim_{\eta \to 0^+} G_{ii}(E + i\eta)$, and $G_{ii}(Z) = [Z - \varepsilon_i - S_i(Z)]^{-1}$ is the diagonal Green's function.²⁴ D(E) is thus given generally by

$$D(E) = \pi^{-1} \lim_{\eta \to 0^+} \int_{-\infty}^{+\infty} dE_i \int_{-\infty}^{+\infty} d\Delta_i \int_{-\infty}^{+\infty} d\varepsilon_i \frac{\eta + \Delta_i}{(E - \varepsilon_i - E_i)^2 + (\eta + \Delta_i)^2} F(E_i, \Delta_i) P(\varepsilon_i) .$$
(2.11)

If E corresponds to a localized state then $\Delta_i \propto \eta \rightarrow 0+$, whence (2.11) reduces to

$$D(E) = \int_{-\infty}^{+\infty} d\varepsilon f_0(E - \varepsilon) P(\varepsilon) .$$
(2.12)

From (2.9b) we thus have

$$M(0) = D(E), \ \mu \to 0+$$
 (2.13)

[Note that $M(Z) \neq D(E+Z)$ for $Z \neq 0$, as $f_0(E_i)$ depends implicitly on E.]

We now consider the $\mu \rightarrow 0+$ behavior of $\hat{f}(k)$, Eq. (2.9a), and restrict ourselves henceforth to three-dimensional sys-

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tems, for which D(E) is nonsingular. Provided V(R) falls off at large R more rapidly than R^{-3} , and provided E is not very close to the band edges of the density of states, the behavior of the Z integral in (2.9a) is dominated by its $Z \rightarrow 0$ behavior and $\hat{f}(k)$ asymptotically approaches

$$\hat{f}(k) \sim \exp\left\{4\pi\rho D(E) \int_{0}^{+\infty} dR \ R^{2}g_{0}(R) \int_{-\infty}^{+\infty} dZ \left[\exp\left[\frac{ik |V(R)|^{2}\mu}{Z^{2}}\right] - 1\right]\right\}.$$
(2.14)

The case $V(R) \sim R^{-3}$, corresponding to dipolar excitons, requires a more subtle analysis which will be described elsewhere; this reflects the fact that dipolar excitons are believed never to be strictly localized at any finite density.^{1,10,11} The restriction that *E* is not arbitrarily close to the band edges ensures that M(Z) has no singularities on the real axis, so that the *Z* integral in (2.9a) is dominated by its $Z \rightarrow 0$ behavior. [That (2.14) yields the $\mu \rightarrow 0+$ limit of $\hat{f}(k)$ under the conditions specified may be verified by direct calculation with a specific V(R).]

With the substitution $u = Z[k\mu | V(R) |^2]^{-1/2}$, and using

$$\int_{-\infty}^{+\infty} du [\exp(i/u^2) - 1] = -(2\pi)^{1/2}(1-i) ,$$

(2.14) reduces to

$$\hat{f}(k) \sim^{\mu \to 0+} \exp[-(1-i)(2\pi k\mu)^{1/2} D(E) J_1(\rho)], \quad (2.15)$$

where

$$J_1(\rho) = 4\pi\rho \int_0^{+\infty} dR \ R^2 g_0(R) | V(R) | \quad .$$
 (2.16)

Note that V(R) must indeed decay more rapidly than

 R^{-3} for the integral (2.16) to converge.

Taking the inverse Fourier transform of (2.15) leads to the following asymptotic behavior for $f(\Delta)$:

$$f(\Delta) \sim \gamma \Delta^{-3/2} \exp(-\pi \gamma^2 / \Delta)$$
, (2.17a)

where

$$\gamma = \mu^{1/2} J_1(\rho) D(E)$$
 (2.17b)

Note that while the mean value of Δ obtained directly from (2.17a) is infinite, the function is normalized to unity and has a well-defined most probable value $\Delta_m(\mu)$, given by

$$\Delta_m(\mu) = \frac{2\pi}{3} \gamma^2(\mu) \propto \mu, \quad \mu \to 0 + \quad . \tag{2.17c}$$

We now consider the asymptotic behavior of $f(\Delta)$ in the $\mu \rightarrow \infty$ limit where the dephasing time scale $\tau = \hbar/2\eta$ becomes extremely small. When dealing for example with low-temperature electronic transport in dirty metals, this corresponds to a situation where, e.g., inelastic electronphonon interactions lead to extremely rapid dephasing. In this limit Eq. (2.9a) asymptotically approaches

$$\widehat{f}(k) \stackrel{\mu \to \infty}{\sim} h(k/\mu) = \exp\left\{4\pi\rho \int_0^{+\infty} dR \ R^2 g_0(R) \left[\exp\left[\frac{ik |V(R)|^2}{\mu}\right] - 1 \right] \right\},$$
(2.18)

where we use the fact that M(Z) is normalized to unity. The resultant most probable value, $\Delta_m(\mu)$, of $f(\Delta)$ is given by that nontrivial solution of $\partial_{\Delta} f(\Delta) = 0$, i.e.,

$$0 = \int_{-\infty}^{+\infty} dk \ k \ \exp[-ik \Delta(\mu)] h(k/\mu); \ \mu \to \infty ,$$
(2.19a)

for which $f(\Delta)$ takes on its largest value. Note from (2.18) that as $\mu \to \infty$, $\hat{f}(k)$ viewed as a function of k and μ depends simply on k/μ . Thus, defining $Z = k/\mu$ and $\Delta' = \mu \Delta(\mu)$, (2.19a) reduces to

$$0 = \int_{-\infty}^{+\infty} dZ \, Z \, \exp(-iZ\Delta')h(Z) , \qquad (2.19b)$$

an equation for Δ' which is independent of μ . It follows immediately that

$$\Delta_m(\mu) = \frac{\Delta'}{\mu}, \quad \mu \to \infty \tag{2.20}$$

where Δ' is *independent* of μ . Equation (2.20) thus gives the explicit μ dependence of $\Delta_m(\mu)$ as $\mu \to \infty$. As an estimate of Δ' we take $\Delta' \simeq \mu \langle \Delta(\mu) \rangle$ $=\mu \lim_{k\to 0} [-i\partial_k h(k/\mu)]$, which yields

$$\Delta' \simeq J_2(\rho) = 4\pi\rho \int_0^{+\infty} dR \ R^2 g_0(R) | V(R) |^2 . \quad (2.21)$$

Having specified the asymptotic behavior of $\Delta_m(\mu)$ in the large- and small- μ limits, we now stress a general symmetry property of $\Delta_m(\mu)$. The real and imaginary parts of the self-energy of atom *i* as given by (2.5) are, respectively, an even and odd function of μ . From (2.6b) we thus see that $f(\Delta;\mu)=f(-\Delta;-\mu)$ where the μ dependence of *f* is made explicit (equivalently, from (2.9a) with the μ dependence of \hat{f} explicit, $[\hat{f}(k;\mu)]^* = \hat{f}(-k;\mu) = \hat{f}(k;-\mu)$). It therefore follows that, quite generally

$$\Delta_m(\mu) = -\Delta_m(-\mu), \quad \forall \mu . \tag{2.22}$$

Consequently, if $\Delta_m(\mu)$ is an analytic function of μ for small μ , then it is an odd function of μ , i.e.,

$$\Delta_m(\mu) \stackrel{\mu \to 0}{\sim} c_1 \mu + c_2 \mu^3 + O(\mu^5) . \qquad (2.23)$$

We have so far established the following asymptotic behavior:

$$\Delta_m(\mu) \stackrel{\mu \to 0}{\sim} T(\rho; E) \mu , \qquad (2.24a)$$

$$\Delta_m(\mu) \stackrel{\mu \to \infty}{\sim} J_2(\rho) \mu^{-1} , \qquad (2.24b)$$

where

$$T(\rho; E) = \frac{2\pi}{3} [J_1(\rho)D(E)]^2 . \qquad (2.25)$$

To analyze (2.9a) in detail beyond these limits is numerically feasible, although complex analytically, requiring specification of a particular V(R) and $P(\varepsilon)$, and a detailed knowledge of M(Z) [via solution of the nonlinear integral equation (2.10) for $\hat{f}_0(k)$]. To interpolate between the established large and small μ limits of $\Delta_m(\mu)$ we therefore employ the simple Padé approximant

$$\Delta_m(\mu) = \frac{T(\rho; E)\mu}{1 + T(\rho; E)J_2^{-1}(\rho)\mu^2} .$$
(2.26)

Note that, in addition to yielding the limiting behavior of (2.24), this approximant has the necessary virtue of reproducing correctly the small μ analytic structure embodied in (2.23).

Equation (2.26) gives the most probable value of the distribution $f(\Delta)$ for (the imaginary part of) the selfenergy of atom *i*. Self consistency is now enforced by requiring that the most probable value of this distribution be equal to the most probable value $\Delta_m = \mu - \eta$ of the self-energies of all other atoms $j \neq i$. Thus, setting $\mu = \eta + \Delta_m$ in (2.26), we obtain the following selfconsistent algebraic equation for Δ_m :

$$\Delta_m = \frac{T(\rho; E)(\eta + \Delta_m)}{1 + T(\rho; E)J_2^{-1}(\rho)(\eta + \Delta_m)^2} .$$
 (2.27)

Equation (2.27) is the central result of this section and will be examined systematically in the remainder of the paper, beginning with the $\eta \rightarrow 0+$ regime corresponding to the absence of dephasing interactions.

Before proceeding further, we note that an approximate solution to the integral equation (2.10) for $\hat{f}_0(k)$ has been given in Ref. 11 for the $\mu \rightarrow 0+$ limit. In the case of lateral disorder alone $[P(\varepsilon)=\delta(\varepsilon-\varepsilon_0)]$ this leads to the following form¹¹ for $f_0(E_i)$:

$$f_{0}(E_{i}) = \begin{cases} \frac{\alpha(E)\pi^{-1}}{\alpha^{2}(E) + (E_{i} - \frac{1}{2}\tilde{E})^{2}}, & \tilde{E}^{2} \le 4J_{2} \\ \delta(E_{i} - x_{0}(E)), & \tilde{E}^{2} \ge 4J_{2} \end{cases},$$
(2.28a)

where $\widetilde{E} = E - \varepsilon_0$ and

$$\begin{aligned} \alpha(E) &= \frac{1}{2} [4J_2(\rho) - \tilde{E}^2]^{1/2} ,\\ 2x_0(E) &= \tilde{E} \mp [\tilde{E}^2 - 4J_2(\rho)]^{1/2} ; \end{aligned} \tag{2.28b}$$

the upper (lower) root in $x_0(E)$ refers to $\tilde{E} > 0$ ($\tilde{E} < 0$). Together with (2.12) this leads to the following expression¹¹ for the density of states D(E) in the $\mu \rightarrow 0+$ limit:

$$D(E) = \begin{cases} \frac{2}{\pi} \left[\frac{1}{4J_2(\rho)} \right] [4J_2(\rho) - \tilde{E}^2]^{1/2}, & \tilde{E}^2 \le 4J_2 \\ 0, & \tilde{E}^2 \ge 4J_2 \end{cases}.$$
(2.28c)

(2.28c) is a familiar semielliptic Hubbard density of states²⁴ with bandwidth $B = 2J_2^{1/2}(\rho)$, and will be employed in specific applications in the following sections.

III. DISCUSSION

A. Anderson localization

In this section we examine the behavior of $\Delta_m \equiv \Delta_m(\eta;\rho;E)$ in the limit of a vanishing dephasing rate, i.e., the limit $\eta \rightarrow 0+$. This corresponds to the "pure" Anderson problem, and the method here developed enables us to investigate the localization-delocalization transition as it is approached from either domain.

For $\eta = 0$, the self-consistency equation (2.27) reduces to

$$\Delta_m(0;\rho;E) = \frac{T\Delta_m(0;\rho;E)}{1 + TJ_2^{-1} [\Delta_m(0;\rho;E)]^2} .$$
(3.1)

Note that $T(\rho; E)$ and $J_2(\rho)$ are necessarily positive. Thus, for ρ or E such that T < 1, the only solution to (3.1) is $\Delta_m = 0$, corresponding to Anderson localized states. From (2.25), the condition $T(\rho; E) = 1$ becomes

$$\frac{2\pi}{3}J_1^2(\rho)D^2(E) = 1 . \qquad (3.2)$$

For given ρ , the critical energies $E_c^{\pm}(\rho)$ for which (3.2) is satisfied yield the upper and lower mobility edges separating regions of localized and extended states. Equivalently, for given *E*, the critical density $\rho_c(E)$ for which (3.2) is satisfied yields the density at which the chosen energy is a mobility edge; in particular for E=0, $\rho_c(0)\equiv\rho_A$ gives the Anderson transition density.

For (ρ, E) such that T > 1, $\Delta_m(0; \rho; E)$ is finite corresponding to the regime of extended states, and is given from (3.1) by

$$\Delta_m(0;\rho;E) = \left(\frac{[T(\rho;E)-1]J_2(\rho)}{T(\rho;E)}\right)^{1/2}, \quad T \ge 1 . \quad (3.3)$$

Assuming $T(\rho; E)$ to be analytic in ρ as $\rho \rightarrow \rho_c(E)$ and in E as $E \rightarrow E_c^{\pm}(\rho)$ (3.3) yields

$$\Delta_m(0,\rho;E) \stackrel{\rho \to \rho_c}{\sim} c(\rho - \rho_c)^s, \quad \rho \ge \rho_c$$

$$E \to E_c^{\pm}$$
(3.4a)

$$\Delta_m(0;\rho;E) \stackrel{-}{\sim} b_{\pm} | E_c^{\pm} - E | {}^{s'}, \quad E_c^{-} \le E \le E_c^{+}$$
(3.4b)

with exponents $s = \frac{1}{2} = s'$ and

$$C = \left[\frac{\partial T}{\partial \rho}\right]_{\rho_c}, \quad b_{\pm} = \left[\frac{\partial T}{\partial E}\right]_{E_c^{\pm}}.$$
 (3.4c)

Note that the localization transition is here predicted continuous, in agreement with the scaling theory of localization.⁶ This is at variance with the conclusions of Girvin and Jonson^{13,14} based on a numerical study of localization on a Bethe lattice, although it is not unambiguously clear that the statistics in Ref. 14 point to a discontinuous transition.

To illustrate the above results we consider explicitly the simple exponential transfer-matrix element

$$V(R) = -V_0 \exp(-R/a_H) . (3.5a)$$

This form is applicable both to a discussion of triplet electronic excitons in (for example) the impurity band of mixed organic crystals, or to a discussion of electronic transport in disordered materials; in the latter case a_H is an effective Bohr radius for the electron under consideration. For simplicity we consider the case of pure lateral disorder alone $[P(\varepsilon)=\delta(\varepsilon)]$ with a perfectly random spatially uncorrelated system for which $g_0(R)=1$. The integrals (2.16) and (2.21) may be evaluated yielding

$$J_1(\rho^*) = 8\pi V_0 \rho^* ,$$

$$J_2(\rho^*) = \pi V_0^2 \rho^* ,$$
(3.5b)

where $\rho^* = \rho a_H^3$ is a reduced (dimensionless) density. We take D(E) to be given by the approximate form (2.28c), whence the instability condition (3.2) reduces to

$$\frac{32}{3\pi}(4\pi\rho^* - \xi^2) = 1 , \qquad (3.5c)$$

where $\xi = E/V_0$ is a reduced energy. For $\xi = 0$, (3.5c) yields the Anderson density, for which

$$\rho_A^{1/3} a_H = 0.29 \ . \tag{3.5d}$$

This falls well within the domain of previously estimated values of $\rho_A^{1/3}a_H$ for exponential transfer-matrix elements, a partial summary of which is given in Ref. 11 and which range from ~0.1 to 0.37. We also note that for uncompensated semiconductors, the critical impurity concentration necessary for a metal-insulator transition is found empirically to satisfy $\rho^{1/3}a_H \approx 0.26$, ²⁵ with which our estimate is in reasonable agreement.

Mobility-edge trajectories for the exponential transfermatrix element are given directly from (3.5c) by

$$\xi_c^{\pm}(\rho^*) = \pm 2\pi^{1/2}(\rho^* - \frac{3}{128})^{1/2}, \quad \rho^* \ge \rho_A^* = \frac{3}{128} \quad . \tag{3.6}$$

[We add, however, that in accordance with the discussion following equation (2.14), (3.6) may not locate mobility edges well when they lie close to the band edges of D(E).] For ξ such that $\xi_c^-(\rho^*) < \xi < \xi_c^+(\rho^*)$, states at the chosen ρ^* are extended; equivalently, from (3.5c), we see that for $\rho^* > \rho_c^*(\xi) = (3\pi + 32\xi^2)/128\pi$ states at the chosen energy are extended. In the regime of extended states, $\Delta_m(0,\rho^*;\xi)$ is given from (3.3) by

$$V_0^{-1}\Delta_m(0;\rho^*;\xi) = (\pi\rho^*)^{1/2} \left[1 - \frac{3\pi}{32(4\pi\rho^* - \xi^2)} \right]^{1/2},$$

$$\rho^* \ge \rho_c^*(\xi) . \quad (3.7)$$

The above results for the exponential transfer-matrix element are illustrated in Fig. 1(a) where we plot $V_0^{-1}\Delta_m$ as a function of ρ^* for the three different energies $\xi=0$,

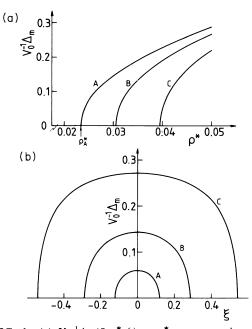


FIG. 1. (a) $V_0^{-1}\Delta_m(0;\rho^*;\xi)$ vs ρ^* as appropriate to the exponential transfer-matrix element (3.5a), and for the three energies $\xi = 0$ (A), 0.3 (B), and 0.45 (C). The Anderson transition density is marked by an arrow. (b) $V_0^{-1}\Delta_m(0;\rho^*;E)$ vs ξ for three different densities $\rho^* = 1.05\rho_A^*$ (A), 1.28 ρ_A^* (B), and $2\rho_A^*$ (C).

0.3, and 0.45, and in Fig. 1(b) where we show $V_0^{-1}\Delta_m$ as a function of ξ for three different densities $\rho^* / \rho_A^* = 1.05$, 1.28, and 2.

We note that the analysis given here is quite readily extended in two directions.

(i) The influence of the static structure of the system upon the localization characteristics can be investigated by employing a more realistic structural correlation function $g_0(R)$. For example, even if one uses merely the lowdensity limit of $g_0(R)$ appropriate to a hard-sphere fluid with hard-sphere diameter d, one can assess the relative influence of the competing length scales a_H and d in determining the metal-insulator transition density (see, e.g., Refs. 11 and 26).

(ii) The effects of band structure on the localization characteristics may be incorporated into the problem. As discussed in Ref. 12, these effects stem from the irreducible many-body interactions neglected in the second-order renormalized perturbation-series expression for the self-energy, Eq. (2.1). Incorporation of such interactions leads to the simple transfer-matrix element V_{ij} being replaced by an effective transfer-matrix element $^{12} \phi_{ij}(\rho; E)$, which is spatially screened or antiscreened according to the region of energy and density under consideration. This in turn leads, 12 for example, to an asymmetry in the mobility-edge trajectories which is not observed in the present level of formulation, as is evident from (3.6) where the mobility-edge trajectories are symmetric in energy about $\xi=0$.

Finally in this section, we wish to comment on the infinite-time behavior of $\langle \langle P_{ii}(t) \rangle \rangle$, the ensemble-averaged

probability that an excitation created on site *i* at time t = 0 will be found on that site at time *t*. As is well known,²⁷ $\langle \langle P_{ii}(\infty) \rangle \rangle$ is given by

$$\langle\!\langle P_{ii}(\infty) \rangle\!\rangle = \left\langle\!\!\left\langle \sum_{\alpha} |C_i^{(\alpha)}|^4 \right\rangle\!\!\right\rangle,$$
 (3.8)

where $C_i^{(\alpha)}$ is the coefficient of the site orbital $|i\rangle$ in the expansion of the (normalized) stationary state of the tight-binding Hamiltonian with energy E_{α} . Only localized states of energy E_{α} give a nonvanishing contribution to the sum in (3.8), as $C_i^{(\alpha)}$ is nonzero only if atom *i* participates in a localized state of energy E_{α} . (In fact $C_i^{(\alpha)}$ is of order $N^{-1/2}$ if particle *i* participates in a state localized on N sites, an observation which forms the basis for use of the inverse participation ratio,²⁸ $L_{\alpha} = \sum_i |C_i^{(\alpha)}|^4$, as a criterion for the existence or otherwise of localized states.) As shown by Thouless,²⁷ for localized states $|C_i^{(\alpha)}|^2$ is given by

$$|C_{i}^{(\alpha)}|^{2} = \left\{1 + \lim_{\eta \to 0+} \left[\Delta_{i}(\eta; E_{\alpha})/\eta\right]\right\}^{-1}, \qquad (3.9)$$

where the η and E_{α} dependence of Δ_i is made explicit, so that (3.8) reduces to

$$\langle\!\langle P_{ii}(\infty)\rangle\!\rangle = \lim_{\eta \to 0+} \left\langle\!\!\left\langle \sum_{\alpha} \frac{|C_i^{(\alpha)}|^2}{1 + \eta^{-1} \Delta_i(\eta; E_{\alpha})} \right\rangle\!\!\right\rangle \,. \tag{3.10}$$

The diagonal Green's function $G_{ii}(E+i\eta)$ is related to the $\{C_i^{(\alpha)}\}$ by²⁷

$$G_{ii}(E+i\eta) = \sum_{\alpha} \frac{|C_i^{(\alpha)}|^2}{E - E_{\alpha} + i\eta} , \qquad (3.11)$$

and thus the density of states for a given realization of the system, $\hat{N}_i(E) = -\pi^{-1} \operatorname{Im} G_{ii}^{(+)}(E)$, is given by

$$\hat{N}_{i}(E) = \sum_{\alpha} |C_{i}^{(\alpha)}|^{2} \delta(E - E_{\alpha}) .$$
(3.12)

The ensemble-averaged density of states $\langle\langle \hat{N}_i(E) \rangle\rangle$ will in general be denoted by N(E); in accordance with the usage prevalent in Sec. II B we shall employ the notation D(E) for the ensemble-averaged density of states only if states of energy E are localized.

With (3.12), Eq. (3.10) reduces to

$$\langle\!\langle P_{ii}(\infty)\rangle\!\rangle = \lim_{\eta \to 0+} \int_{-\infty}^{+\infty} dE \left\langle\!\!\left\langle \frac{\hat{N}_i(E)}{1 + \eta^{-1} \Delta_i(\eta; E)} \right\rangle\!\!\right\rangle ,$$
(3.13)

which is exact. If now we make the approximation of replacing Δ_i by its most probable value, $\Delta_m(\eta; E)$, Eq. (3.13) reduces simply to

$$\langle\!\langle P_{ii}(\infty) \rangle\!\rangle \simeq \lim_{\eta \to 0+} \int_{E_{-}}^{E_{+}} dE \frac{D(E)}{1 + \eta^{-1} \Delta_{m}(\eta; E)} ,$$
 (3.14)

where E_{\pm} are the band edges of D(E). Equation (3.14) may also be obtained rather more directly from the exact expression due to Economou and Cohen²⁹

$$\langle\!\langle P_{ii}(\infty)\rangle\!\rangle = \lim_{\eta \to 0+} \frac{\eta}{\pi} \int_{-\infty}^{\infty} dE \langle\!\langle |G_{ii}(E+i\eta)|^2\rangle\!\rangle ,$$
(3.15a)

which is equivalent to (3.8). By replacing $\Delta_i(\eta; E)$ in $G_{ii}(Z)$ by its most probable value, $\Delta_m(\eta; E)$, (3.15a) reduces to

$$\langle\!\langle P_{ii}(\infty)\rangle\!\rangle \simeq \lim_{\eta \to 0+} \int_{-\infty}^{\infty} dE \int_{-\infty}^{\infty} dE_i \int_{-\infty}^{\infty} d\varepsilon_i \frac{(\eta + \Delta_m)\pi^{-1}}{(E - \varepsilon_i - E_i)^2 + (\eta + \Delta_m)^2} \frac{1}{1 + \eta^{-1}\Delta_m} P(\varepsilon_i) f_0(E_i) . \tag{3.15b}$$

The only nonzero contributions to (3.15b) come from localized states, for which $\Delta_m(\eta; E) \propto \eta$ as $\eta \rightarrow 0+$, whence (3.15b) reduces precisely to (3.14) with D(E) given by (2.12). With a knowledge of both D(E) and $\Delta_m(\eta; E)$ (for all E), Eq. (3.14) constitutes a simple and practical prescription for estimating $\langle\!\langle P_{ii}(\infty) \rangle\!\rangle$.

There is, however, one general aspect of the preceding discussion that we wish to stress. From the exact expressions (3.8) or (3.13), and also from (3.14), it is clear that only states of energy E which are localized contribute to $\langle\langle P_{ii}(\infty)\rangle\rangle^{27}$ Note then that all localized states in the band contribute to $\langle\langle P_{ii}(\infty)\rangle\rangle$. It follows that $\langle\langle P_{ii}(\infty)\rangle\rangle = 0$ only if all states in the band are extended. We define the density ρ_D such that $\langle\langle P_{ii}(\infty)\rangle\rangle \to 0$ as $\rho \to \rho_D$ from below. ρ_D does not, of course, correspond to the insulator-metal transition density ρ_M . The latter occurs when states at the Fermi energy E_F become extended; in particular, if N(E) is symmetric in $E, E_F = 0$, and the insulator-metal transition density ρ_A . As ρ is increased

above ρ_M , a progressively larger fraction of states in the band become extended, i.e., the mobility edges move progressively towards the band edges. As $\rho \rightarrow \rho_D > \rho_M$, all states in the band become extended, and thus $\langle\langle P_{ii}(\infty) \rangle\rangle \rightarrow 0$. We mention this because Loring and Mukamel^{30,31} have recently developed an approximate mode-coupling theory of quantum percolation,³⁰ and also an effective dephasing theory for the optical analogue of an Anderson metal-insulator transition;³¹ both theories are based on a tight-binding description. In each case, however, Loring and Mukamel conflate the critical disorder required to delocalize all states in the band with the critical disorder required to induce an insulator-metal transition. This is clearly incompatible with the above general remarks, and its validity would seem questionable.

B. Dephasing interactions

In this section we examine the general η dependence of Δ_m as given by solution of the self-consistency equation

(2.27), in order to investigate the interplay between dephasing and localization.

The problem is simplified by defining the reduced variables $\tilde{\eta}$ and $\tilde{\Delta}_m$ given by

$$\tilde{\eta} = \eta J_2^{-1/2}(\rho)$$
, (3.16a)

$$\widetilde{\Delta}_m(\widetilde{\eta};\rho;E) = \Delta_m(\eta;\rho;E) J_2^{-1/2}(\rho) . \qquad (3.16b)$$

Equation (2.27) thus simplifies to

$$\widetilde{\Delta}_{m} = \frac{T(\rho; E)(\widetilde{\eta} + \widetilde{\Delta}_{m})}{1 + T(\rho; E)(\widetilde{\eta} + \widetilde{\Delta}_{m})^{2}} , \qquad (3.17)$$

where we note that the entire ρ and E dependence of $\overline{\Delta}_m$ is contained in the function $T(\rho; E)$ given by (2.25), i.e., $\overline{\Delta}_m(\tilde{\eta}; \rho; E) \equiv \overline{\Delta}_m(\tilde{\eta}; T)$. We wish to solve (3.17) for $\overline{\Delta}_m$ given $\tilde{\eta}$, ρ , and E (or $\tilde{\eta}$ and T) as input; in particular, we are interested in the $\tilde{\eta}$ dependence of $\overline{\Delta}_m$ for given ρ and E. Equation (3.17) is a cubic equation for $\overline{\Delta}_m$, the physical solution of which, with given $T(\rho; E)$ and a real positive $\tilde{\eta}$, is necessarily real and positive. A convenient means of analyzing (3.17) is to note that it is a quadratic in $\tilde{\eta}$ with solution

$$\tilde{\eta} = \frac{1 \pm [1 - 4T^{-1}(\rho; E) \tilde{\Delta}_m^2]^{1/2}}{2 \tilde{\Delta}_m} - \tilde{\Delta}_m , \qquad (3.18)$$

and with the roots chosen such that both $\overline{\Delta}_m$ and $\overline{\eta}$ are real and positive. Analysis of the problem thus resolves itself into two principal domains.

(1) $0 \le T(\rho; E) < 2$: for $0 \le \tilde{\eta} \le \tilde{\eta}_{max} = [2 - T(\rho; E)]/2[T(\rho; E)]^{1/2}$, the negative root of (3.18) is appropriate, while for $\tilde{\eta} \ge \tilde{\eta}_{max}$ the positive root is chosen. As discussed below, this domain may be subdivided further into the regions $0 \le T \le 1$ and 1 < T < 2.

(2) $T(\rho; E) \ge 2$: here only the positive root of (3.18) is ever appropriate. The physical significance of the classification will be discussed shortly, after describing the $\tilde{\eta}$ dependence of $\tilde{\Delta}_m$ characteristic of each of the three $T(\rho; E)$ intervals.

1. Region 1a: $0 \le T(\rho:E) \le 1$

For $\eta = 0$, this region corresponds to the regime of Anderson localized states, as described in Sec. III A. For $T(\rho; E) \leq 1$ the general $\tilde{\eta}$ dependence of $\tilde{\Delta}_m$ (or equivalently Δ_m versus η) is shown as case A of Fig. 2; the specific example is for T=0.9. As η is increased from zero, Δ_m increases from zero through a maximum, $\Delta_{m,\max}$, occurring at η_{\max} (as indicated by an arrow), decreasing thereafter with increasing η to the asymptotic form

$$\widetilde{\Delta}_{m}(\widetilde{\eta};\rho;E) \stackrel{\widetilde{\eta}\to\infty}{\sim} \widetilde{\eta}^{-1}$$
(3.19a)

or

$$\Delta_m(\eta;\rho;E) \stackrel{\eta \to \infty}{\sim} J_2(\rho)\eta^{-1} . \tag{3.19b}$$

The small- η behavior of Δ_m may be quantified by considering the small- η behavior of (3.18). For $T(\rho; E) < 1$ [with the negative root of (3.18)] this leads to

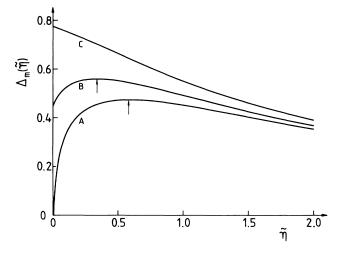


FIG. 2. $\tilde{\Delta}_m(\eta;\rho;E)$ vs $\tilde{\eta}$ as obtained from solution of Eq. (3.18) for $T(\rho;E)=0.9$ (A), 1.25 (B), and 2.5 (C). The maximum $\tilde{\Delta}_m$ for cases A and B is indicated by an arrow. Case A corresponds to a regime of zero-temperature Anderson localized states, and case B illustrates the domain of incipient localization or weak delocalization.

$$\Delta_m(\eta;\rho;E) \stackrel{\eta \to 0}{\sim} \frac{T(\rho;E)}{1 - T(\rho;E)} \eta + O(\eta^3), \quad T < 1 .$$
 (3.20a)

Similarly, for $T(\rho; E) = 1$, (3.18) yields

$$\widetilde{\Delta}_{m}(\widetilde{\eta};\rho_{c};E) \stackrel{\widetilde{\eta}\to 0}{\sim} \widetilde{\eta}^{1/3}, \quad T(\rho;E) = 1 , \qquad (3.20b)$$

or equivalently, $\Delta_m(\eta;\rho_c;E) \sim [J_2(\rho_c)\eta]^{1/3}$. For η infinitesimally small, (3.20a) is precisely the behavior associated with localized states, and (3.20b) gives the $\eta \rightarrow 0+$ behavior of Δ_m at $T(\rho; E) = 1$, i.e., for $\rho_c(E)$ at given E or for $E_c^{\pm}(\rho)$ at given ρ . For given $T(\rho; E) < 1$ and with η finite, (3.20a) is valid in a range of η such that $\widetilde{\Delta}_m(\widetilde{\eta}) \ll \widetilde{\Delta}_{m,\max} = [T(\rho; E)]^{1/2}/2$. For η finite we thus see from Fig. 2 or Eq. (3.20) that dephasing effects lead to erstwhile localized states of energy E becoming extended, and that Δ_m increases linearly with η for small η . In dealing for example with low-temperature electronic transport, one expects η to be an increasing function of temperature,^{13,14} so that Δ_m is itself an increasing function of temperature at sufficiently low temperatures. Under these circumstances the mechanism of electronic conduction is phonon-assisted transport between zero-temperature Anderson localized states.

2. Region 1b: $1 < T(\rho; E) < 2$

For $\eta = 0$ this region corresponds to a regime in which states of energy E are extended, such that $\Delta_m(0;\rho;E) \equiv \Delta_m^0$ is finite and given by (3.3). For $1 < T(\rho;E) < 2$ the general η dependence of Δ_m is shown as case **B** of Fig. 2, the specific example being for $T(\rho;E)=1.25$. As η increases from zero, Δ_m increases monotonically from Δ_m^0 through a maximum $\Delta_{m,\max}$ occurring at η_{\max} (as indicated on the figure), decreasing thereafter with increasing η to the large η asymptotic form (3.19). With the exception that $\Delta_m(0;\rho;E)$ is finite, the qualitative behavior of Δ_m versus η is the same as that of region 1a; in particular $\widetilde{\Delta}_m$ goes through a maximum, although we note that $\widetilde{\eta}_{\max}$ shifts progressively towards zero as T increases towards $T(\rho;E)=2$. The small- η behavior of Δ_m in this region will be quantified below.

3. Region 2: $T(\rho; E) \ge 2$

As with region 1b, $\Delta_m(0;\rho;E)$ is finite corresponding to a domain of $\eta = 0$ delocalized states of energy E. In contrast to regions 1a and 1b, however, $\Delta_m(\eta;\rho;E)$ decreases monotonically with increasing η from Δ_m^0 [given by (3.3)] at $\eta = 0$ to the asymptotic form (3.19); the maximum value of $\Delta_m(\eta;\rho;E)$ thus occurs at $\eta = 0$. This behavior is shown as case C of Fig. 2 for the specific value $T(\rho;E)=2.5$.

For regions 1b and 2, then, $\Delta_m(0;\rho;E)$ is finite corresponding to extended states of energy E for $\eta=0$. For the case of electronic transport, and considering in particular $E=E_F$ (the Fermi energy), regions 1b and 2 correspond to zero-temperature metallic behavior. In contrast, region 1a is a zero-temperature insulating domain. The low-temperature (small- η) behavior in the two regions corresponding to states which are extended for $\eta=0$, can be found from (3.18). In both cases $(1 < T < 2 \text{ and } T \ge 2)$ it is found that $\Delta_m(\eta;\rho;E) - \Delta_m(0;\rho;E)$ is linear in η for small η , i.e.,

$$\Delta_m(\eta;\rho;E) = \Delta_m^0 + C_{\Delta}\eta + \cdots, \quad T(\rho;E) > 1 , \quad (3.21a)$$

where Δ_m^0 is given by Eq. (3.3). The coefficient C_{Δ} is given by

$$C_{\Delta} = \frac{1}{2} \frac{2 - T(\rho; E)}{T(\rho; E) - 1}, \quad T(\rho; E) > 1$$
 (3.21b)

Thus, for $1 < T(\rho; E) < 2$ (region 1b), Δ_m initially increases with increasing η from its $\eta = 0$ value, Δ_m^0 ; whereas for region 2 $[T(\rho; E) \ge 2] \Delta_m$ decreases with increasing η from Δ_m^0 at $\eta = 0$. The condition $T(\rho; E) = 2$ therefore corresponds to a crossover point in the low-temperature behavior of $\Delta_m(\eta; \rho; E)$, from a Δ_m which initially increases with increasing temperature (region 1b) to one which decreases as the temperature is increased from zero (region 2). This crossover behavior is central to the discussion of Mooij correlation¹⁸ given in the following section.

Note further from Eqs. (3.20a) and (3.21b) that the low-temperature behavior of Δ_m for regions 1a $[T(\rho; E) < 1]$ and 1b $[1 < T(\rho; E) < 2]$ are both such that Δ_m initially increases with increasing temperature—from zero at $\eta = 0$ in the former case, and from $\Delta_m^0 \neq 0$ in the latter. It is on account of this behavior that we have classified both regimes together as region 1. Region 1b is thus the domain of "incipient localization" or "weak delocalization" in that, although states of energy E are extended at T=0 K, they are sufficiently weakly delocalized that the effects of incipient localization are manifest in the low-temperature behavior of Δ_m , where inelastic dephasion.

ing interactions lead to an initial increase in Δ_m as the temperature is increased from zero.

We now refer briefly to the large- η asymptotic behavior of Δ_m , which is given by (3.19) for all regions. This corresponds to the limit of incoherent transport (large dephasing) with a small dephasing time scale, $\tau = \hbar/2\eta$, a regime usually treated via a Pauli master equation approach.³²⁻⁴⁰ From Eqs. (2.3b) or (2.5b), the probability that an electron initially on site *i* will escape outwards in unit time, given by²⁷ $2\hbar^{-1}\Delta_i$, reduces to $2\hbar^{-1}\sum_j' |V_{ij}|^2/\eta$ as $\eta \to \infty$, i.e., the hopping rate from site *i* to *j* is $2 |V_{ij}|^2/\eta\hbar$, as inherent in approaches to the incoherent limit based on a master equation description.

To illustrate the discussion of this section we consider the simple example discussed in Sec. III A, namely the exponential transfer matrix element (3.5a) under conditions of pure lateral disorder, and for a perfectly random spatially uncorrelated system. For this example $T(\rho^*;\xi) = 32(4\pi\rho^* - \xi^2)/3\pi$ where ρ^* and ξ are the reduced variables defined previously. We consider a fixed density, $\rho^* = \frac{5}{2}\rho_A^* = \frac{15}{256}$. For $\eta = 0$ (zero temperature) the mobility edges are given from (3.6) by $\xi_c^{\pm}(\rho^*) = \pm 0.665$; states of energy $\xi > \xi_c^+$ or $\xi < \xi_c^-$ are localized, while states such that $\xi_c^- < \xi < \xi_c^+$ are extended. Confining ourselves for convenience to the lower half band $(\xi < 0)$, case A of Fig. 2 $[T(\rho^*;\xi)=0.9]$ corresponds to $\xi=-0.687$ and represents a zero-temperature localized state. For this situation the low-temperature behavior of Δ_m is given from (3.20a) by $\tilde{\Delta}_m \sim 9\tilde{\eta}$, and electronic transport is due to phonon-assisted tunneling between zero-temperature Anderson localized states. Case C of Fig. 2 [$T(\rho^*;\xi)=2.5$] corresponds to extended midband ($\xi = 0$) states, far from the mobility edges; for this case, $\tilde{\Delta}_m(0;\rho^*;\xi) \equiv \tilde{\Delta}_m^0 = (\frac{3}{5})^{1/2}$, and the low-temperature behavior of Δ_m is given from (3.21) by $\widetilde{\Delta}_m \sim \widetilde{\Delta}_m^0 - \frac{1}{6} \widetilde{\eta}$ or, equivalently, $\tilde{\Delta}_m / \tilde{\Delta}_m^0 \sim 1 - 0.215 \tilde{\eta}$. For extended states far from the mobility edges, low-temperature transport is predominantly bandlike, due to coherent propagation interrupted by random inelastic electron-phonon interactions which act to diminish Δ_m as the temperature is increased from zero. In contrast, case B of Fig. 2 $[T(\rho^*;\xi)=1.25]$ corresponds to $\xi=-0.607$ and represents a state which, while extended, is sufficiently weakly delocalized that the effects of incipient localization are clearly recognizable in the low-temperature behavior of Δ_m . From (3.21) this is given by $\tilde{\Delta}_m \sim \tilde{\Delta}_m^0 + \frac{3}{2}\tilde{\eta}$ with $\tilde{\Delta}_m^0 = 5^{-1/2}$, or $\tilde{\Delta}_m / \tilde{\Delta}_m^0 \sim 1 + 3.35\tilde{\eta}$. The positive temperature coefficient of $\tilde{\Delta}_m$ in the region of extended states just before the onset of localization reflects the increase in electronic mobility due to phonon-assisted tunneling caused by dynamical electron-phonon interactions.^{13,14} For a given small temperature (fixed η), the relative importance of the phonon-assisted transport over the zerotemperature Δ_m^0 contribution increases as $\xi \rightarrow \xi_c^-$ from above (or $\xi \rightarrow \xi_c^+$ from below), i.e., as $T(\rho^*;\xi) \rightarrow 1+$. For $T(\rho^*;\xi) = 1.05$ ($\xi = -0.653$), example, with $\widetilde{\Delta}_m / \Delta_m^0 \sim 1 + 43 \widetilde{\eta}.$

The above remarks may also be illustrated by considering the density dependence of Δ_m for a fixed energy and for a variety of different η 's. In the context of our specific

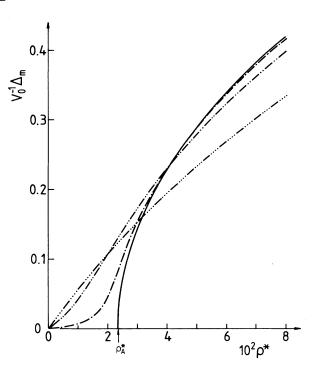


FIG. 3. $V_0^{-1}\Delta_m(\eta;\rho^*;\xi)$ vs ρ^* for the exponential transfermatrix element (3.5a), at the fixed energy $\xi=0$ and for (i) $\eta=0$ (-----), (ii) $V_0^{-1}\eta=0.01$ (-·-), (iii) $V_0^{-1}\eta=0.075$ (-·--), and (iv) $V_0^{-1}\eta=0.3$ (-···-). The $\eta=0$ curve corresponds to case A of Fig. 1(a), and the Anderson transition density ρ_4^* is indicated by an arrow.

example this is shown in Fig. 3, where we plot $V_0^{-1}\Delta_m$ versus ρ^* at the fixed energy $\xi=0$ and for $V_0^{-1}\eta=0$, 0.01, 0.075, and 0.3. The $\eta=0$ curve corresponds to case A of Fig. 1(a), and ρ_A^* is the Anderson transition density at which $\xi=0$ is a mobility edge and such that for $\rho^* > \rho_A^*$ states at $\xi=0$ are extended. For finite temperatures ($\eta\neq 0$) the concept of a mobility edge is of course ill defined and the pristine $\eta=0$ transition is smeared out. It is however clear that the effects of zero-temperature localization and weak delocalization are apparent at sufficiently low temperatures.

Finally, for the purposes of simplicity, an implicit assumption in the preceding discussion is that all temperature dependences are contained in the dephasing variable η . This is not generally correct; temperature dependences will in addition enter the problem via both a phononrenormalized transfer matrix element and a dependence of the pair distribution function $g_0(R)$ on temperature. Although omitted in the preceding discussion, such effects are readily incorporated into the theory.

C. Electronic transport in dirty metals and Mooij correlation

Some years ago Mooij¹⁸ observed a striking correlation in many disordered materials between the temperature coefficient of resistivity (TCR) and the residual resistivity $1/\sigma_0$. For weakly disordered ("clean") metals with small residual resistivities, the TCR is positive, reflecting an increased resistive scattering from phonons as the temperature is raised. For strongly disordered ("dirty") metals, however, the situation is frequently reversed. Mooij¹⁸ found that as the resistivity increases, the TCR decreases, and becomes negative for systems with residual resistivities greater than 150 $\mu\Omega$ cm. He concluded furthermore that this behavior was universal, independent of material composition, and holding for both disordered crystalline and amorphous systems.

Much theoretical attention has since been devoted to the problem; for recent reviews see Refs. 4, 5, and 41. In particular, recent work^{13,14,19,42-45} has sought to explain the phenomenon from the standpoint of Anderson localization or incipient localization. An explanation along these lines was first proposed by Jonson and Girvin,^{13,14} who pointed out that for large disorder the static phonon approximation fails, and in the region of weakly extended states close to the onset of localization dynamic electronphonon interactions cause an increase in electronic mobility due to phonon-assisted tunneling. In this section we examine the Mooij correlation in the context of our present theory. In addition we comment on the frequently cited universality of the threshold resistivity, an aspect of the problem addressed very recently by Tsuei.¹⁹

To obtain an estimate for the dc conductivity in the strong disorder regime, we follow essentially the procedure described in the Appendix to Ref. 14. Consider the familiar relation, due to Thouless,⁴⁶ for the conductance G(L) of a cube of side L:

$$\frac{e^2}{2\hbar} \frac{\Delta E(L)}{\delta E(L)} = G(L) = \sigma(L)L \quad . \tag{3.22a}$$

 $\delta E(L)$ is the mean spacing of the cube's energy levels, and $\Delta E(L)$ the mean of the fluctuation in the energy levels consequent upon a change in boundary conditions from periodic to antiperiodic; $G(L) = \sigma(L)L$ defines the conductivity, which is independent of L in the Ohmic regime. $\delta E(L)$ is given by

$$\delta E(L) = \left[\frac{a}{L}\right]^3 \frac{1}{N(E_F)} , \qquad (3.22b)$$

where $a = \rho^{-1/3}$ (ρ is the number density of particles) and $N(E_F)$ is the density of states per site at the Fermi energy. For strong disorder, $\Delta E(L) = \hbar/t_L$,⁴⁶ where $t_L = L^2/D$ is the time taken for an electron to diffuse a distance L and D is the electronic diffusion constant. The time $\tau_l = l^2/D$ for an electron to travel a distance of the order of the mean free path $l \sim a$ is given by $\tau_l = \hbar/2\Delta_m(\eta;\rho; E_F)$, whence $t_L = (L/a)^2 \hbar/2\Delta_m(\eta;\rho; E_F)$. The conductivity is thus given by

$$\sigma = \frac{e^2}{\hbar a} N(E_F) \Delta_m(\eta; \rho; E_F) . \qquad (3.23)$$

Before discussing the starting equation (3.23), we note that it differs from that derived in Ref. 14 in one significant respect. Instead of Δ_m appearing in (3.23), Girvin and Jonson¹⁴ have $\eta + \langle \Delta \rangle$, where $\langle \Delta \rangle$ is the ensemble-averaged imaginary part of the electron selfenergy (more precisely the forward-hopping self-energy, as their analysis was performed on a site-diagonally disordered Cayley tree). The form $\sigma = (e^2/\hbar a)N(E_F)(\eta$ $+\langle\Delta\rangle$) cannot, however, be correct; for if the transfermatrix elements V_{ij} are set to zero, transport cannot occur and the conductivity should be zero: that this is not the case for the above expression is clear, since for $V_{ij}=0$, $\langle\Delta\rangle=0$ but $N(E_F)$ is still in general well defined. We stress, however, that this criticism applies solely to the result in the Appendix of Ref. 14. The central analytical expressions derived by Girvin and Jonson do conform correctly to the $V_{ij}=0$ limit. To estimate the dc conductivity we take

To estimate the dc conductivity we take $N(E_F) \simeq D(E_F)$, which is tantamount to assuming that the density of states at the Fermi energy is fairly insensitive to whether states there are localized or weakly extended. Thus

$$\sigma \simeq \frac{e^2}{\hbar a} D(E_F) \Delta_m(\eta; \rho; E_F) , \qquad (3.24)$$

which we expect to provide a reasonable estimate in the dirty limit. The η (temperature) dependence of Δ_m (and hence σ) has been discussed in detail in Sec. III B. The region $1 < T(\rho; E_F) < 2$ is the regime of weak delocalization and is illustrated as case B of Fig. 2. As seen from the figure, σ initially increases with increasing temperature from the residual value σ_0 $\simeq (e^2/\hbar a) D(E_F) \Delta_m(0,\rho;E_F)$ at zero temperature; this is the negative TCR regime. As temperature is increased further, σ goes through a maximum and decreases slowly thereafter with increasing temperature, corresponding to a positive TCR. Note further that as $\Delta_m^0 \equiv \Delta_m(0;\rho;E_F)$ decreases, the initial temperature slope of $\Delta_m(\eta;\rho;E_F)$ increases, i.e., as the residual resistivity σ_0^{-1} increases the TCR becomes progressively more negative, in harmony with experimental observation.^{18,19,47} In contrast, as $T(\rho; E_F)$ increases progressively towards the value 2, Δ_m^0 progressively increases and the TCR becomes less negative. For $T(\rho; E_F) > 2$, as shown in Fig. 2, Δ_m is a decreasing function of temperature; this corresponds to the usual positive TCR behavior. The crossover behavior in the temperature dependence of σ thus occurs at $T(\rho; E_F) = 2$ (for which $\Delta_m^0 = [J_2(\rho)/2]^{1/2}$), i.e., for

$$\frac{\pi}{3} [J_1(\rho) D(E_F)]^2 = 1 , \qquad (3.25a)$$

with a resultant crossover residual conductivity $\sigma_{0,c}$ given by

$$\sigma_{0,c} \simeq \frac{e^2}{\hbar a} \left[\frac{\dot{3}}{2\pi} \right]^{1/2} \frac{J_2^{1/2}(\rho)}{J_1(\rho)} . \qquad (3.25b)$$

Equations (3.25a) and (3.25b) together determine the threshold residual resistivity $\sigma_{0,c}^{-1}$. With explicit expressions for $D(E_F)$ and $J_1(\rho)$, Eq. (3.25a) determines the material parameters required for crossover behavior to occur at the chosen $a = \rho^{-1/3}$, and with a further knowledge of $J_2(\rho)$, Eq. (3.25b) then determines $\sigma_{0,c}$. It is evident that $D(E_F)$, $J_1(\rho)$, and $J_2(\rho)$ all depend on the material characteristics of the system. From (2.16) or (2.21), for example, we see that the band integrals J_1 and J_2 depend on the particular choice of transfer matrix element, and on the pair distribution function of the system which in

turn reflects the structural characteristics of the specific disordered material. This is of particular relevance, for as recently stressed by Tsuei,¹⁹ a threshold residual resistivity of $\sigma_{0,c}^{-1} = 150 \ \mu\Omega$ cm has often been ascribed fundamental significance as a universal boundary which divides the positive and negative TCR regimes. From analysis of extensive experimental data, however, Tsuei¹⁹ has shown that the threshold resistivity is not universal, that it depends on material characteristics and can have a wide range of values from ~30-500 \ \mu\Omega cm and above. This conclusion was also presaged to some extent by Nagel.⁴⁷

To illustrate the above remarks we consider a system with both site-diagonal and topological disorder present. We take the distribution of site energies to be a Lorentzian

$$P(\varepsilon) = \frac{\lambda \pi^{-1}}{\lambda^2 + (\varepsilon - \varepsilon_0)^2} , \qquad (2.26a)$$

where the half-width λ characterizes the degree of diagonal disorder. D(E) is given by (2.12) with $f_0(E_i)$ given by solution of the integral equation (2.10) for $\mu = 0$, an approximate solution of which is given in Ref. 11. This leads to the following expression for D(E) at the Fermi energy $E_F = \varepsilon_0$,

$$D(E_F) = \frac{2\pi^{-1}}{\lambda + [\lambda^2 + 4J_2(\rho)]^{1/2}} , \qquad (2.26b)$$

which reduces correctly to (2.28c) for $\lambda = 0$. Equations (3.25), which together determine the threshold residual conductivity, thus simplify to

$$\frac{2J_1(\rho)}{(3\pi)^{1/2} \{\lambda + [\lambda^2 + 4J_2(\rho)]^{1/2}\}} = 1 , \qquad (3.27a)$$

$$\sigma_{0,c} \simeq \frac{e^2}{\hbar a} \frac{1}{2^{1/2} \pi} \frac{2J_2^{1/2}(\rho)}{\lambda + [\lambda^2 + 4J_2(\rho)]^{1/2}} .$$
(3.27b)

With specified forms for the transfer-matrix element and pair distribution function, J_1 and J_2 may be evaluated from (2.16) and (2.21). As a specific example we consider the exponential transfer-matrix element (3.5a) with a simple pair distribution function $g_0(R) = \Theta(R - d)$ where d is a hard-sphere diameter. The integrals J_1 and J_2 are here given by

$$J_{1} = 4\pi V_{0} \left[\frac{a_{H}}{a} \right]^{3} \left[\left[\frac{d}{a_{H}} \right]^{2} + 2\frac{d}{a_{H}} + 2 \right] \exp(-d/a_{H}) ,$$

$$J_{2} = \pi V_{0}^{2} \left[\frac{a_{H}}{a} \right]^{3} \left[2 \left[\frac{d}{a_{H}} \right]^{2} + 2\frac{d}{a_{H}} + 1 \right] \exp(-2d/a_{H}) ,$$
(3.28)
$$\exp(-2d/a_{H}) ,$$

and reduce to (3.5b) for d = 0. For this example, (3.27a) with (3.28) interrelates $a = \rho^{-1/3}$, the structural parameters d and a_H , and the degree of diagonal disorder λ , which are required for threshold behavior; (3.27b) gives the threshold residual conductivity.

To obtain a numerical estimate for $\sigma_{0,c}$ we consider the case of lateral disorder alone ($\lambda=0$) for which (3.27b)

 $0 \rightarrow 0$

reduces generally and simply to

$$\sigma_{0,c} \simeq \frac{0.23e^2}{\hbar a}, \quad \lambda = 0$$
 (3.29a)

It should of course be remembered that a and the structural parameters required for crossover are interconnected by

$$\frac{J_1(\rho)}{[3\pi J_2(\rho)]^{1/2}} = 1, \quad \lambda = 0$$
(3.29b)

[which depends on the particular V(R) and $g_0(R)$], so that $\sigma_{0,c}$ is dependent on material characteristics. Turning to (3.29a) we note that this estimate for the threshold residual conductivity is considerably larger than Mott's minimum metallic conductivity,^{4,5,48} $\sigma_{\min} \simeq 0.03e^2/\hbar a$, which appears to hold experimentally.^{4,19} For *a* in the region ~1.5-4 Å, (3.29a) yields a threshold resistivity of ~250-700 $\mu\Omega$ cm, which we regard as reasonable agreement with the experimental situation.¹⁹ Note further from (3.27b) that with site diagonal disorder included, the threshold residual conductivity will be less than the $\lambda=0$ estimate (3.29a), as one expects physically.

Finally, we consider the expression (3.23) for σ in the zero-temperature $(\eta=0)$ limit. The behavior of $\Delta_m(0;\rho;E)$ as the localization transition is approached

from the regime of extended states has been described in Sec. III A [see Eqs. (3.3) and (3.4)]. Extrapolation of (3.23) down to the metal-insulator transition suggests

$$\sigma \sim \operatorname{const} \times (\rho - \rho_c)^s , \qquad (3.30)$$

with a mean-field critical exponent $s = \frac{1}{2}$, and similarly $\sigma \sim \text{const} \times |E_c^{\pm} - E|^{1/2}$ as $E \rightarrow E_c^{\pm}$ for the *E* dependence of the conductivity. This mean-field result differs from the generally accepted exponent s = 1 for three-dimensional systems, obtained from various scaling approaches to the problem^{2-4,6,7} (although we note that the original scaling theory⁷ predicted s < 1). However, as stressed recently by Kramer *et al.*³ and Mott and Kaveh,⁵ the correct exponent cannot be said to be known with certainty, and we shall not comment further here on the problem.

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