Some aspects of impurity conduction

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To study diffusion and localization of electrons in impurity bands, the self-consistent current relaxation theory is applied to Wegner's local gauge-invariant model for random hopping transport. The approach covers both the conducting and the insulating phase for arbitrary dimensionality d within a single framework. Explicit results for the mobility, the static polarizability, and the frequency-dependent conductivity are given for $d=2$ and 3. For $d=2$, an abrupt transition from a state of strong localization to a weakly localized quasimetallic phase is found. Scaling laws for the conductivity near the mobility edge are worked out and the role of the upper critical dimensionality $d=4$ is discussed.

I. INTRODUCTION

Electron-transport processes due to random hopping are of considerable interest, since they are the underlying phenomenon of impurity conduction in semiconductors (see Ref. 1). For the transport properties of such disordered systems the occurrence of Anderson localization is crucial.[2] It implies that either the whole band consists of localized states, or mobility edges exist that separate regions of localized states from regions of extended ones.[3] Anderson localization has been studied for different models with a variety of techniques (see, e.g., Ref. 4). To examine hopping transport due to spatially fluctuating overlap of localized electron wave functions, Anderson's original work was extended by considering a random kinetic energy in addition to a random chemical potential.[5]

An extreme case of random hopping was considered by Wegner.[6] In his model the electron tunneling matrix elements are distributed symmetrically around zero. As a result the system exhibits local gauge invariance: Phase coherence is destroyed completely by going from one lattice point to another. So local gauge invariance is the precise mathematical formulation of Mott's random-phase-model assumption.[1] The impurity-band model with local gauge invariance does not have any small parameter, and this makes it plain why a transport theory for strongly disturbed systems is so difficult. To proceed, Wegner extended the model by introducing n electronic orbitals per site. He demonstrated that the correlation functions of interest can be calculated exactly in the limit $1/n \to 0$. This observation provided the basis for a systematic $1/n$ expansion.[7] Thereby, the leading correction in $1/n$ to the conductivity was calculated; in particular the resistance correction of two-dimensional systems was found to be divergent, in accordance with the corresponding result obtained originally for the Edwards model.[8] By a Lagrangian formulation[9] contact was made also to a nonlinear σ model for which renormalization-group calculations have been performed.[10]

To proceed beyond perturbation analysis of the conductivity the self-consistent current-relaxation theory (SCCR) was proposed.[11] SCCR made it possible to obtain transport coefficients and excitation spectra above and below the mobility edge within one approximation framework. For the Edwards model of disordered conductor mobilities, localization lengths and dynamical conductivities were calculated. The theory was extended to study also random hopping within a continuum model.[12] However, in this work certain approximations made at the very beginning prevented us from studying narrow impurity bands.

In this paper, previous work[11,12] will be extended to calculate transport properties of Wegner's[6] model. We discuss scaling at the metal-insulator transition, mobility-edge positions, conductivity, and polarizability for all dimensionalities d and number of orbitals n. Expanding our results in terms of $1/n$ and $1/(d-2)$, we compare our approximations to the exact results obtained before[6,7] for the metallic phase.

II. PRELIMINARIES

In this section we introduce notations and outline some general concepts necessary for the following calculations. The particle positions $\vec{r},\vec{s},\ldots$, are restricted to the N sites of a d-dimensional hypercubic lattice with lattice constant a. The n orbitals will be labeled by $\alpha,\beta,\ldots$. Let us emphasize that we are mainly interested in the case $n=1$ as a model for an impurity band well separated from other bands. However, since our method works at the same expense no matter how large n is, we study the general case to get in contact with previous work.[6,7] With $a^{\dagger}_{\vec{r}\alpha}, a_{\vec{r}\alpha}$ denoting fermion creation and annihilation operators, respectively, the Hamiltonian reads

$$H=\frac{1}{\sqrt{n}}\sum_{\vec{r},\vec{s},\alpha,\beta} h^{\alpha\beta}_{\vec{r}\vec{s}}\, a^{\dagger}_{\vec{r}\alpha} a_{\vec{s}\beta}\ . \tag{2.1}$$

So electron-electron interaction is neglected. The hopping amplitudes $h^{\alpha\beta}_{\vec{r}\vec{s}}$ are real random variables. They are distributed independently apart from the hermiticity requirement $h^{\alpha\beta}_{\vec{r}\vec{s}}=h^{\beta\alpha}_{\vec{s}\vec{r}}$. The distribution is assumed to be

symmetrical around zero. Thus h and $-h$ occur with the same weight. Hence, $\langle h^{\alpha\beta}_{\vec{r}\vec{s}}\rangle_a=0$, and the canonical transformation $a_{\vec{r}\alpha}\to\sigma_{\vec{r}\alpha}a_{\vec{r}\alpha}$, where $\sigma_{\vec{r}\alpha}=\pm1$, maps H onto a Hamiltonian entering ensemble averages $\langle\ \rangle_a$ with equal weight. This property is Wegner's local gauge invariance.[6] Consequently, $\langle h_{12}h_{34}\rangle_a=0$ unless $1=4$ and $2=3$, or $1=3$ and $2=4$, where the obvious abbreviation $1=(\vec{r}_1,\alpha_1)$, etc., was used. Restricting the discussion to nearest-neighbor (NN) hopping, the model is specified by two parameters, ϵ and t,

$$\langle h_{12}h_{34}\rangle_a=(\delta_{14}\delta_{23}+\delta_{13}\delta_{24}-\delta_{12}\delta_{13}\delta_{14})f_{\vec{r}_1\vec{r}_2}\ , \tag{2.2a}$$

$$f_{\vec{r}\vec{s}}=\begin{cases}\epsilon^2 & \text{if } \vec{r}=\vec{s}\\ t^2 & \text{if } \vec{r} \text{ NN of } \vec{s}\end{cases}\ . \tag{2.2b}$$

For $n=1$, ϵ is the spread of the local chemical potential's distribution (diagonal disorder), while t is the spread of the tunneling matrix elements (off-diagonal disorder). Note that due to gauge invariance there is no coherent tunneling.

For a discussion of particle propagation in disordered systems two variables are of central importance: $\rho(\vec{q})$ and $j(\vec{q})$ denoting density and longitudinal current-density fluctuations, respectively, with wave vector $\vec{q}$. $\rho(\vec{q})$ is the Fourier transform of the density operator field,

$$\rho(\vec{r})=\sum_\alpha (a^\dagger_{\vec{r}\alpha}a_{\vec{r}\alpha}-\langle a^\dagger_{\vec{r}\alpha}a_{\vec{r}\alpha}\rangle)\ , \tag{2.3a}$$

$$\rho(\vec{q})=\frac{1}{\sqrt{N}}\sum_{\vec{r}} e^{-i\vec{q}\cdot\vec{r}}\rho(\vec{r})\ , \tag{2.3b}$$

where the $\vec{q}$ are restricted to the first Brillouin zone. $\langle\ \rangle$ denotes, here and in the following, quantum-mechanical expectation values. Defining the Liouville operator $\mathscr{L}$ acting on dynamical variables A as usual, $\mathscr{L}A=[H,A]$, one obtains a continuity equation $\mathscr{L}\rho(\vec{q})=-qj(\vec{q})$, which serves to define $j(\vec{q})$. Explicitly one finds

$$j(\vec{q})=\frac{1}{q}\frac{1}{(nN)^{1/2}}\sum_{1,2}h_{12}(e^{-i\vec{q}\cdot\vec{r}_1}-e^{-i\vec{q}\cdot\vec{r}_2})a^\dagger_1a_2\ . \tag{2.4}$$

The homogeneous current density will be denoted by $j=j(q=0)$.

As done before,[11] transport properties will be described with the help of Kubo functions[13] or propagators, $\Phi_{AB}(z)=(A\mid(\mathscr{L}-z)^{-1}\mid B)$. Here the scalar product in the space of dynamical variables is given by averaged thermodynamic compressibilities for zero temperature,

$$(A\mid B)=\lim_{T\to0}\left\langle\int_0^{1/T}d\lambda[\langle A^\dagger B(i\lambda)\rangle-\langle A^\dagger\rangle\langle B\rangle]\right\rangle_a\ . \tag{2.5}$$

The density propagator reads

$$\Phi(\vec{q},z)=(\rho(\vec{q})\mid(\mathscr{L}-z)^{-1}\mid\rho(\vec{q}))\ , \tag{2.6}$$

and the homogeneous current propagator is given by

$$K(z)=(j\mid(\mathscr{L}-z)^{-1}\mid j)\ . \tag{2.7}$$

The causal functions $\Phi_{AB}(z)$ are determined by their absorptive parts

$$\Phi''_{AB}(\omega)=[\Phi_{AB}(\omega+i0)-\Phi_{AB}(\omega-i0)]/2i$$

by a Hilbert-Stieltjes transformation

$$\Phi_{AB}(z)=\int_{-\infty}^{\infty}d\omega\,\pi^{-1}\Phi''_{AB}(\omega)/(\omega-z)\ .$$

In particular, the frequency-dependent conductivity is obtained by the absorptive part of the current propagator as follows[13]:

$$\sigma(\omega)=e^2K''(\omega)\ , \tag{2.8}$$

where e is the particle charge. The density propagator can be rewritten in the form

$$\Phi(\vec{q},z)=-g(\vec{q})[z+K(\vec{q},z)/g(\vec{q})]^{-1}\ ,$$

where

$$g(\vec{q})=(\rho(\vec{q})\mid\rho(\vec{q}))$$

is the density compressibility and $K(\vec{q},z)$ denotes some causal kernel with positive spectrum. Because of the continuity equation one gets for $q\to0$ the long-wavelength asymptote

$$K(\vec{q},z)\left[\sum_i\sin^2(q_ia)\right]^{-1}\to K(z)/a^2\ .$$

Hence, one can write the generalized hydrodynamic approximation $\Phi(\vec{q},z)\cong\Phi^H(\vec{q},z)$, where

$$\Phi^H(\vec{q},z)=-g(\vec{q})\left[z+\left[\sum_i\sin^2(q_ia)\right]\frac{K(z)}{g(\vec{q})a^2}\right]^{-1}\ . \tag{2.9}$$

Since $g(q\to0)=\rho_F$, with ρ_F denoting the density of states at the Fermi energy ϵ_F, the formula reduces for $q\to0$ to the Green-Kubo identity. So Eq. (2.9) generalizes the Green-Kubo equation such that the exact $q\neq0$ compressibility and the lattice symmetry is taken care of.

We now note some known results for later reference. The averaged one-particle Green function

$$\langle G_{12}(z)\rangle_a=\langle\langle 1\mid(H-z)^{-1}\mid 2\rangle\rangle_a$$

is diagonal due to local gauge invariance: $\langle G_{12}(z)\rangle_a=\delta_{12}G(z)$. Applying a simple decoupling procedure to the self-energy of $G(z)$, one obtains

$$G(z)=\frac{1}{2U^2}[-z+(z^2-4U^2)^{1/2}]\ , \tag{2.10a}$$

$$U^2=\epsilon^2+2dt^2\ . \tag{2.10b}$$

Equation (2.10a) is the self-consistent Born-approximation result for the Green function, which has been used before in another context.[14] For the density of states $\rho_F=nG''(\omega=\epsilon_F)/\pi$ it yields a semicircle,

$$\rho_F=\frac{n}{\pi U}[1-(\epsilon_F/2U)^2]^{1/2}\Theta(4U^2-\epsilon_F^2)\ . \tag{2.11}$$

Such a result follows also for well-separated impurity bands from the coherent-potential approximation.[15]

The representation of the propagators

$$\Phi_{1234}(z)=(a_1^\dagger a_2 \mid (\mathscr{L}-z)^{-1} \mid a_3^\dagger a_4)$$

in terms of Green functions reads, for bilinear Hamiltonians,

$$\Phi_{1234}(z)=\int_{-\infty}^{\infty}\frac{d\omega_1}{\pi}\int_{-\infty}^{\infty}\frac{d\omega_2}{\pi}\frac{\Theta(\epsilon_F-\omega_1)-\Theta(\epsilon_F-\omega_2)}{(z-\omega_1+\omega_2)(\omega_1-\omega_2)}\times\langle G''_{13}(\omega_1)G''_{42}(\omega_2)\rangle_a \ . \tag{2.12}$$

The exact Eq. (2.12) reveals a peculiar symmetry due to time reversal invariance: For a real Hamiltonian, we have $G''_{12}(\omega)=G''_{21}(\omega)$ and consequently $\Phi_{1234}=\Phi_{3214}=\Phi_{1432}$, which was proven diagramatically in Ref. 7. Actually, this symmetry is the very reason for the known anomalies[8] in $d=2$, as was pointed out in a paper by Gorkov *et al.*[16]

A standard approximation for the conductivity $\sigma(\omega)$ consists of factorizing the ensemble average in Eq. (2.12). With the help of Eqs. (2.2), (2.4), and (2.7) we find a Mott-Hindley formula,[17]

$$\sigma^{(0)}(\omega)=ne^2 2a^2t^2\phi^{(0)\prime\prime}(\omega) \ , \tag{2.13a}$$

$$\phi^{(0)}(z)=\frac{1}{n^2}\int_{-\infty}^{\infty}\frac{d\omega}{\omega-z}\int_{-\infty}^{\infty}dx\rho\left[x-\frac{\omega}{2}\right]\rho\left[x+\frac{\omega}{2}\right]\frac{1}{\omega}\times\left[\Theta\left[\epsilon_F-x+\frac{\omega}{2}\right]-\Theta\left[\epsilon_F-x-\frac{\omega}{2}\right]\right] , \tag{2.13b}$$

where $\rho(\omega)=nG''(\omega)/\pi$ is the density of states with energy ω. In particular, the dc conductivity is given by the density of states squared,

$$\sigma^{(0)}=n\,2\pi a^2t^2(\rho_F/n)^2 \ . \tag{2.13c}$$

For the present model the f-sum rule

$$\alpha_F=\int_{-\infty}^{\infty}d\omega\,\pi^{-1}\sigma(\omega)/e^2 \ ,$$

which enters the following theory as the current compressibility $\alpha_F=(j \mid j)$ depends on the disorder. Substitution of $\sigma^{(0)}$ instead of σ yields

$$\alpha_F=\frac{8}{3}\frac{n}{\pi U}a^2t^2\left[1-\left[\frac{\epsilon_F}{2U}\right]^2\right]^{3/2} \ . \tag{2.14}$$

Wegner has shown[6] that the preceding results for ρ_F, $\sigma(\omega)$, and α_F are exact in the limit $1/n\to 0$. Notice that the conductivity $\sigma^{(0)}(\omega)$ exhibits two frequency scales, $2U-\epsilon_F$ and $2U+\epsilon_F$, rather than a single one as in Drude theory.

Some general remarks concerning the nature of transport in the local gauge-invariant model may be in order. The transition rate for an electron's hop from one lattice site to a neighboring one, calculated by the golden rule, is $1/\tau=2\pi t^2\rho_F/n$. Making the assumption of random walk, the diffusivity reads $D=a^2/\tau$ and Einstein's relation $e^2D=\sigma^{(0)}/\rho_F$ yields

$$\sigma^{(0)}=2\pi a^2t^2\rho_F{}^2/n \ .$$

So the Mott-Hindley results[17] are not a consequence of the random-phase assumption alone, but, in addition, one has to assume a Markovian process. Now we have to wonder whether the random-walk hypothesis is justified. Indeed, for a two-step process the two hops are uncorrelated because of the model's random-phase property. There is, however, one exception: If the second step reverses the first one, one gets on averaging, the average of the squared transition amplitude rather than the squared average. A similar observation holds for multistep processes as well. So there is just one class of processes for which the random-walk hypothesis does not hold, and this class represents the quantum-interference contribution to the conductivity.[8] In the limit $n\to\infty$ the weight of these processes tends to zero as $1/n$, and this is the reason why our simple argument leading to $\sigma^{(0)}$ yields the exact result in this limit. The random-walk model does not exhibit mobility edges: $\sigma^{(0)}\neq 0$ whenever $\rho_F\neq 0$. These observations have two important consequences. Firstly, the whole task of any transport theory for strongly disordered systems, in particular for impurity bands, consists of going beyond the factorization approximation.[15,17] Secondly, those relaxation processes which, e.g., yield the Boltzmann-equation limit for the conductivity of Anderson's model[2] are completely absent in Wegner's model. The physics of the good conductor in the standard theory of electron transport is utterly different from the physics considered in the limit $1/n\to 0$ in the local gauge-invariant model. Therefore the current-relaxation processes dealt with in the original version of the SCCR (Ref. 11) do not occur for the Hamiltonian studied in the present paper. Nevertheless, the straightforwardly used SCCR deals successfully with the mentioned quantum-interference process, as we will demonstrate in the following sections.

III. APPROXIMATION SCHEME

It has been shown[18] that the density of states for noninteracting electrons is uncritical at the mobility edge. The same can be believed for all static correlations. Therefore we consider it reasonable to replace all static correlations by their lowest-order approximation. In particular, we use the density of states and f-sum rule as given by Eqs. (2.11) and (2.14), respectively, for all values of n.

Application of the Zwanzig-Mori reduction algorithm[19] yields an expression for the current propagator, Eq. (2.7), in terms of the current-relaxation kernel (CRK) $m(z)$,

$$K(z)=-\alpha_F[z+m(z)]^{-1} \ . \tag{3.1}$$

The CRK, which can be interpreted as irreducible self-energy of the current propagator, is given by

$$m(z)=(Q\mathscr{L}j \mid (Q\mathscr{L}Q-z)^{-1} \mid Q\mathscr{L}j)/\alpha_F \ , \tag{3.2a}$$

where $Q=1-\alpha_F^{-1} \mid j)(j \mid$ projects perpendicular to j. The fluctuating force $Q\mathscr{L}j$ is easily found from Eq. (2.4),

$$Q\mathscr{L}j=\frac{i}{n\sqrt{N}}\sum_{1,2,3}h^{\bullet}_{13}h^{\bullet}_{32}(\vec{r}_1+\vec{r}_2-2\vec{r}_3)\vec{e}_1a_1^\dagger a_2 \ . \tag{3.2b}$$

Here $\vec{e}_1$ is the unit vector in the 1 direction [without loss of generality we have chosen $\vec{q}=(q,0,\ldots,0)$]. We have

also applied the factorization approximation

$$(h_{13}h_{32}a_1^\dagger a_2 \mid \rho) \cong \langle h_{13}h_{32}\rangle_a (a_1^\dagger a_2 \mid \rho)$$

so that

$$h_{13}^{\bullet}h_{32}^{\bullet} \equiv h_{13}h_{32} - \langle h_{13}h_{32}\rangle_a \equiv h_{13}^{\bullet\bullet}h_{32}^{\bullet\bullet} ,$$

etc. The fluctuating force is a sum of product modes consisting of fermion excitations $a_1^\dagger a_2$ and of random-field fluctuations $h_{13}h_{32}$. The essential approximation of the theory now consists of factorizing the average of products into products of averages.[11] This procedure may be viewed as a simple version of a mode-coupling approximation,[20]

$$m(z) = [1/(\alpha_F n^2 N)] \sum_{1,2,3,\bar{1},\bar{2},\bar{3}} [(\vec{r}_1 + \vec{r}_2 - 2\vec{r}_3)\cdot\vec{e}_1][(\vec{r}_{\bar{1}} + \vec{r}_{\bar{2}} - 2\vec{r}_{\bar{3}})\vec{e}_1]\langle h_{13}^{\bullet}h_{32}^{\bullet}h_{\bar{1}\bar{3}}^{\bullet\bullet}h_{\bar{3}\bar{2}}^{\bullet\bullet}\rangle_a \Phi_{12\bar{1}\bar{2}}(z) . \tag{3.3}$$

Assuming a Gaussian distribution of the h, the average can be factorized. With the help of Eq. (2.2) the result reads

$$m(z) = M_0(z) + M_1(z) + M_2(z) ,$$

where

$$M_0(z) = [1/(\alpha_F n^2 N)] \sum_{1\neq 2} \sum_{3} f_{\vec{r}_1\vec{r}_3} f_{\vec{r}_3\vec{r}_2} [(\vec{r}_1 + \vec{r}_2 - 2\vec{r}_3)\cdot\vec{e}_1]^2 \Phi_{1212}(z) , \tag{3.4a}$$

$$M_1(z) = [1/(\alpha_F n^2 N)] \sum_{1\neq 2} \sum_{3} f_{\vec{r}_1\vec{r}_3} f_{\vec{r}_3\vec{r}_2} [(\vec{r}_1 + \vec{r}_2 - 2\vec{r}_3)\cdot\vec{e}_1]^2 \Phi_{1221}(z) , \tag{3.4b}$$

$$M_2(z) = [2/(\alpha_F n^2 N)] \sum_{1,3} [2(\vec{r}_1 - \vec{r}_3)\cdot\vec{e}_1 f_{\vec{r}_1\vec{r}_3}]^2 [\Phi_{1111}(z) - \Phi_{1133}(z)] . \tag{3.4c}$$

The significance of the three contributions is quite different. Let us consider the most important term $M_1(z)$ first. Because of the symmetry mentioned in connection with Eq. (2.12) we have

$$\Phi_{1221}(z) = \Phi_{1122}(z) .$$

The latter function is the density propagator for the $n=1$ model; this is also true, apart from uninteresting higher-order corrections in $1/n$, for general n after summation over the orbital indices entering Eq. (3.4b). Hence one gets

$$M_1(z) = \frac{1}{\alpha_F n N} \sum_{\vec{q}} w_1(\vec{q}) \Phi(\vec{q},z) , \tag{3.5}$$

where the vertex reads

$$w_1(\vec{q}) = 4t^2a^2 \left[\cos(q_1 a) \left[\epsilon^2 + 2t^2 \sum_{i=1}^{d} \cos(q_i a) \right] + 2t^2 \sin^2(q_1 a) - 2t^2/n \right] . \tag{3.6}$$

For vanishing q, the vertex approaches a constant, and it is this low-q limit which governs the low-frequency singularities of the decay integral (3.5). Similarly, $M_2(z)$ can be written in the form of Eq. (3.5) with a vertex [correct for $n=1$ and correct apart from higher $(1/n)$ corrections for large n] as follows:

$$w_2(\vec{q}) = (32/n) t^2 a^2 \sin^2(q_1 a/2) . \tag{3.7}$$

So this term merely yields a correction to $w_1(\vec{q})$ in Eq. (3.5) which does not modify the $q=0$ limit of the vertex.

Because of local gauge invariance the mode $a_1^\dagger a_2$ for $1\neq 2$ is perpendicular to the density mode, consisting of sums over $a_3^\dagger a_3$. Thus the modes constituting the propagator $\Phi_{1212}(z)$ in Eq. (3.4a) do not have any overlap with the density mode. The propagator $\Phi_{1212}(z)$ is not critical, neither for the $q\to 0, z\to 0$ singularities nor for the conductor-insulator–transition problem. For these reasons we will not evaluate it self-consistently, but rather replace it by its leading-order factorization approximation. One finds

$$M_0(z) = (n/\alpha_F) 4a^2 t^2 [U^2 - 2t^2/n] \phi^{(0)}(z) , \tag{3.8}$$

where $\phi^{(0)}$ is given in Eq. (2.13b).

IV. RESULTS

A. Self-consistency equations

Let us summarize the equations derived in the preceding sections. The current correlation function $K(z)$ was expressed in terms of a regular kernel $M_0(z)$ and a critical kernel $M(z)$ in the form

$$K(z) = -\alpha_F [z + M_0(z) + M(z)]^{-1} . \tag{4.1}$$

Functions α_F and $M_0(z)$ are given explicitly in Eqs. (2.14) and (3.8), while $M(z)$ is expressed in terms of $\Phi(\vec{q},z)$ as

$$M(z) = \left[4t^2a^2 (U^2 - 2t/n) \frac{\rho_F}{\alpha_F n N} \right] \times \sum_{\vec{q}} \frac{w_1(\vec{q}) + w_2(\vec{q})}{w_1(q=0)\rho_F} \Phi(\vec{q},z) . \tag{4.2}$$

Approximating $\Phi(\vec{q},z)$ by the generalized hydrodynamic form, Eq. (2.9), the preceding results provide a closed set of equations for $M(z)$. For given parameters ϵ, t, and ϵ_F one has to determine those solutions which allow for a spectral representation for $M(z)$ with non-negative spec-

tral function $M''(\omega)$. The preceding results formulate the SCCR theory for the gauge-invariant impurity-band model. The contribution $M(z)$ to the current-relaxation rate, which goes beyond the lowest-order result $M_0''(\omega)$, depends on the density propagator, Eq. (2.9). The latter has to be calculated simultaneously with the rate $M''(\omega)$. Besides the self-consistency requirement there are two further crucial points of the theory.[11] First, approximations are not attempted for the conductivity, but they are attempted for the current-relaxation rate. Second, the rate, and thus the conductivity, are not only considered for zero frequency. The very point of the Anderson transition is the change of an essentially frequency-independent dissipative kernel to a singular, strongly z-dependent reactive function.

The major qualitative difference between the present work and the original discussion of localization within the Edwards model is connected with the long-wavelength asymptotics of the vertex entering Eq. (4.2). In earlier papers,[11] the coupling of the random forces to potential gradients was considered, leading to a vertex proportional to q^2. These gradient contributions are absent in the present model because of the local gauge-invariance property, as discussed in Sec. II. After the discovery of the quantum-interference phenomenon,[8] Prelovsek demonstrated how to handle this new physics within SCCR.[21] Details of this theory for the Anderson transition, in particular a discussion of the interplay of both decay contributions to $M(z)$, have been first worked out in Ref. 22. Most of the work on modern transport theory is based on diagrammatic analysis of perturbation expansions. So it is very interesting that it was also possible to formulate at least parts of the SCCR within this well-established framework.[23] In their first attempt,[23] Vollhardt and Wölfle incorporated the self-consistency requirement as done before within the mode-coupling theory, but recently[4] they have found a novel diagrammatic justification of the old results.[11,22] This observation holds with the reservation that eventually the diagrammatic work will also bring out a proper handling of cutoff problems and vertices for $q\neq 0$. It would certainly also be worthwhile to derive or improve the preceding equations within the diagrammatic approach to the present model.[7]

Because of the generalized hydrodynamic approximation for $\Phi(q,z)$ the self-consistency equations can be rewritten in the compact form[24]

$$\frac{K(z)}{K_0(z)}=1-\mathscr{A}F_d\left[\left[\frac{z\rho_F}{q_0^2K(z)}\right]^{1/2}\right]. \tag{4.3}$$

Here the lowest-order correlation function was introduced,

$$K_0(z)=-\alpha_F[z+M_0(z)]^{-1}.$$

To get dimensionless expressions a scaling wave number q_0 was introduced. The dimensionless coupling constant of the theory reads

$$A=\frac{1}{n}\left[\left[U^2-\frac{2t^2}{n}\right]\frac{1}{t^2}\right]\frac{9d}{d-2}\left\{4q_0a\left[1-\left[\frac{\epsilon_F}{2U}\right]^2\right]\right\}^{-2}, \tag{4.4}$$

and $\mathscr{A}=(d-2)A$. The function $F_d(\zeta)$ is given in terms of the compressibility $g(\vec{q})$ and vertices, Eqs. (3.6) and (3.7), as

$$F_d(\zeta)=\frac{1}{Nd}\sum_{\vec{q}}\left[[w_1(\vec{q})+w_2(\vec{q})]\frac{g(\vec{q})}{w_1(q=0)\rho_F}\right]\times\left[\zeta^2+\left[\sum_i \sin^2(q_ia)/(aq_0)^2\right]\frac{\rho_F}{g(\vec{q})}\right]^{-1}. \tag{4.5}$$

At present it does not seem worthwhile to carry out the cumbersome lattice sum entering the definition of $F_d(\zeta)$. So let us replace the integral over the Brillouin zone by an integral over a sphere of radius $q_0\cong\pi/a$. The integrand will be approximated by its $q\to 0$ asymptote, so that

$$F_d(\zeta)\cong\int_0^1 dk\,k^{d-1}(\zeta^2+k^2)^{-1}. \tag{4.6}$$

B. Critical region

Let us demonstrate that the self-consistency equations describe a conductor-insulator transition. We will do this by working out the asymptotic solution near the transition point.[11] A critical regime is defined implicitly in the space of variables $(\epsilon,t,d,n,\epsilon_F,\omega)$, where $z=\omega+i0$, $\omega\geq 0$, by three requirements. First, frequencies considered have to be so small that the lowest-order conductivity can be replaced by its dc value: $\omega/\nu\ll 1$, where $i\nu=M_0(\omega+i0)$. Thus $K_0=i\sigma_0/e^2$ with $\sigma_0=e^2\alpha_F/\nu$. Second, the critical kernel $M(z)$ shall be considered so large that the true conductivity $K(z)$ is considerably smaller than the lowest-order result: $|K(z)e^2/\sigma_0|\ll 1$. This requirement is necessary to justify the use of the hydrodynamic form for $\Phi(q,z)$. Third, we require the low-frequency polarizability $\chi(z)=e^2K(z)/z$ to be very large:

$$|z\alpha_F/(K(z)\nu^2)|\ll 1.$$

Before simplifying the self-consistency equations under the specified conditions, one has to recognize the following. $d=2$ is a lower marginal dimensionality in the sense that $F_2(\zeta)$ diverges for $\zeta\to 0$. So we will discuss this case separately in Sec. IV F. $d=4$ is an upper critical dimensionality in the sense that the derivative of $F_4(\zeta)$ for $\zeta\to 0$ exhibits a logarithmic divergency. The consequences of the latter singularity will be considered in Sec. IV D. For $2<d<4$ one gets

$$F_d(\zeta)=(d-2)^{-1}-\zeta^{d-2}(\pi/2)/\cos[\tfrac{1}{2}\pi(d-3)]+\cdots,$$

and so Eq. (4.3) can be written as

$$\frac{e^2K(z)}{i\sigma_0}=1-A+\left[\frac{\mathscr{A}(\pi/2)}{\cos[\frac{1}{2}\pi(d-3)]}\right]\times\left[\frac{z\rho_F}{q_0^2K(z)}\right]^{(d-2)/2}+\cdots. \tag{4.3'}$$

We will see that $A\to 1$ is a necessary condition for being in the critical region. So with the separation parameter

$$\tau = A - 1 , \tag{4.7}$$

and with the dimensionless frequency

$$\hat{\omega} = \omega[\nu\rho_F/(\alpha_F q_0^2)] ,$$

one gets for the dimensionless current correlation function $\hat{K} = e^2 K/\sigma_0$, the scaling law

$$\hat{K} = |\tau| S(\hat{\omega}/|\tau|^{2+y}), \quad y = \frac{4-d}{d-2}, \quad 2 < d < 4 . \tag{4.8a}$$

The scaling function $S(\zeta)$ is the causal solution of the equation

$$S(\zeta) = \pm i + i[\pi x/\sin(\pi x)](\zeta/S)^x, \quad x = (d-2)/2 \tag{4.8b}$$

where $\pm$ holds for $\tau \lesseqgtr 0$.

These results obviously imply a conductor phase for $\tau < 0$ and an insulator phase for $\tau > 0$. For the dc conductivity one gets $\sigma = \sigma_0(-\tau)^s$ with exponent $s = 1$. For the polarizability one gets

$$\chi = e^2(\pi x/\sin\pi x)^{1/x}(\rho_F/q_0^2)\tau^{-2\mu} ,$$

where $\mu = (y+1)/2$. The polarizability determines the localization length $r_0^2 = \chi_0/(\rho_F e^2)$ (see subsection D), so that μ is the exponent for the divergence of r_0 near the transition point. In particular one gets $s = \mu(d-2)$. At the edge, there is the critical current spectrum $\sigma(\omega) \sim \omega^{(d-2)/d}$. These results have been obtained before for the Edwards model,[25,22] and they are consistent with those derived by Wegner[26] with renormalization-group techniques. The numerical values of the exponents agree with those found by Oppermann and Wegner[7] for $d - 2 \to 0$.

For $d > 4$ one gets

$$F_d(\zeta) = (d-2)^{-1} - \zeta^2(d-4)^{-1} + \cdots ,$$

and Eq. (4.3) can be rewritten as

$$\frac{K(z)}{i\alpha_F/\nu} = 1 - A + \frac{\mathscr{A}}{d-4}\frac{z\rho_F}{q_0^2 K(z)} + \cdots . \tag{4.3''}$$

So the dimensionless conductivity obeys the scaling law

$$\hat{K} = |\tau| S(\hat{\omega}/\tau^2), \quad d > 4 \tag{4.9a}$$

where the scaling function is the causal solution of the elementary equation

$$S(\zeta) = \pm i - (i/y)(\zeta/S) . \tag{4.9b}$$

In agreement with the predictions obtained within the Edwards model,[22] we find for $d > 4$ the scaling exponents to become independent of the dimensionality. The values $s = 1$, $\mu = \frac{1}{2}$, and the critical current spectrum behavior $\sigma(\omega) \sim \sqrt{\omega}$ for $\tau = 0$, agree with those obtained for the percolation dynamics of the classical Lorentz problem.[24] Our values for the exponents for $d > 4$ agree with those found for Anderson's model on a Bethe lattice,[27] which represents the $d \to \infty$ limit. A number of arguments leading to an upper critical dimensionality $d = 4$ have been given in Ref. 28.

Let us add two further remarks. First, in principle, Eq. (4.3) is capable of describing at $d < 4$ crossover phenomena from Wegner scaling to classical scaling.[22] However, for the discrete model discussed here the crossover point lies outside the range of validity of the scaling laws. Second, our localization criterion $A = 1$ with A given by Eq. (4.4) yields, at the band edges, localized states for all finite d and n for arbitrary disorder. We have found this to be a consequence of local gauge invariance, which would persist if one went beyond the hydrodynamic approximation. In contrast, in an Edwards model for $d > 4$, ϵ must exceed some critical value in order to get any localized states.[22]

C. dc conductivity

We have shown that for $A < 1$ the CRK behaves regularly for $z \to 0$ and our Eq. (4.3) describes a conductor. For $d > 2$, we find in the dc limit,

$$\sigma = \sigma_0(1 - A) . \tag{4.10}$$

The surprising simplicity of this result is a consequence of the hydrodynamic approximation. Taking the full density propagator into account, we would get deviations from Eq. (4.10) outside the critical regime.[24] At the band edges, we have $A > 1$ for any finite n and consequently $\sigma = 0$. For $d > 2$, there can be extended states around the band center, provided the diagonal disorder is not too large compared to the off-diagonal one. Figure 1 exhibits a representative result for a σ-vs-ϵ_F curve, the cross-hatched part of the abscissa indicates the region of localized states.

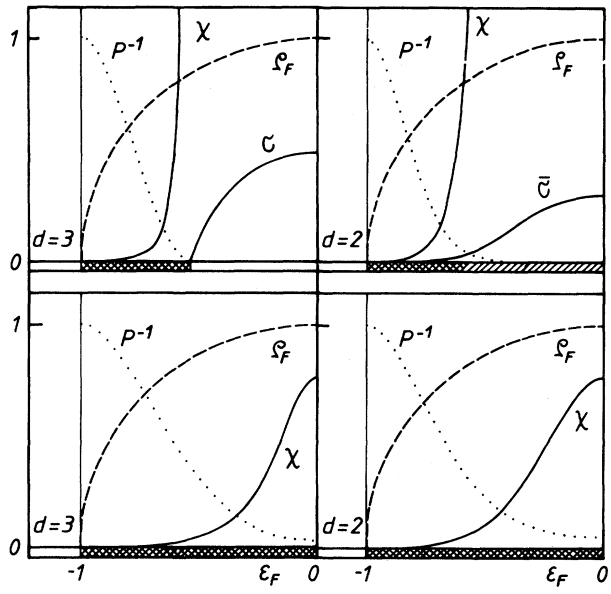

FIG. 1. Density of states ρ_F in units of $1/(2U)$, dc conductivity σ in units of σ_0, low-frequency conductivity $\bar{\sigma} = \sigma(iU/500)$ in units of σ_0, polarizability χ in units of 100 ρ_F/q_0^2, and inverse participation ratio P^{-1} as functions of Fermi energy ϵ_F in units of $2U$ for $d = 2$ and 3. Parameters were chosen as follows (top to bottom): $d = 3$—$\mathscr{A}[1 - (\epsilon_F/2U)^2] = 0.51, 1.20$; $d = 2$—$\mathscr{A}[1 - (\epsilon_F/2U)^2] = 0.19, 0.46$. Hatching and cross hatching indicate weakly and strongly localized regions, respectively. Only half of the band is shown.

For $d \leq 2$, A diverges, and there is no truly metallic phase.[8,7]

Let us notice the following. By approximating

$$[w_1(\vec{q})+w_2(\vec{q})]/w_1(0) \cong 1, \quad g(\vec{q}) \cong \rho_F$$

in Eq. (4.5) we found that there is indeed a regime of mobile states for $d=3$ and $n=1$ if $\epsilon=0$. But we can not overlook the possibility that a better treatment of F_d would imply all states to be localized for $d=3$ and $n=1$. The precise value of the relevant coupling and hence the position of the mobility edge is sensitive with respect to all approximation details. Computer experiments would be very helpful to settle this question.

Regarding Eq. (4.10) as an expansion of the dc conductivity in $1/n$, we identify σ_0 as the contribution of order $(1/n)^0$. It agrees with the exact result $\sigma^{(0)}$, Eq. (2.13c), only apart from a factor $\frac{8}{9}[1-(\epsilon_F/2U)^2]$. This deficiency stems from $\sigma^{(0)}(\omega)$ having two frequency scales, as mentioned in Sec II, while we have approximated the conductivity essentially by a one-parameter curve with the same area. At the band center the two frequency scales merge, and consequently our failure is negligible. Actually, the failure can be removed everywhere in the band at the expense of a slightly more complicated theory. One has to study the CRK's self-energy rather than the CRK itself. However, since for $n=1$ the factorization approximation is a gross overestimation of the conductivity, we believe σ_0 to be not a bad approximation for the regular term in this case. Apart from the same factor, the correction term of order $1/n$ agrees with the exact result.[7]

D. Localization length

The insulator phase is characterized by the kernel $M(z)$ exhibiting a pole $M(z) \sim -1/z$. The static polarizability $\chi = e^2 K(z)/z$, $z \to 0$, is finite. The density correlation function exhibits also a pole $\Phi(q,z) = -f(q)/z$, $z \to 0$, where

$$f(q) = -\rho_F[1+(r_0 q)^2]^{-1} ,$$

and $r_0^2 = \chi/e^2\rho_F$. The δ-function contribution to the density spectrum reflects the nonergodicity of density fluctuations in the insulator phase.[13] Studying the time evolution of the mean-square radius of a density perturbation $S(t) = \langle [\vec{x}(t)]^2 \rangle/(2d)$, one gets for long times $S(t) - S(0) \to r_0^2$ as opposed to Einstein's result for the conductor phase: $S(t) - S(0) \to (\sigma/\rho_F)t$. These general results for the unified description of the conductor-insulator transition have been first considered by one of the authors.[11] Another characterization of the insulator is the inverse participation ratio P^{-1}.[29] Within the SCCR theory it is related to χ, since $P^{-1} = \sum_{\vec{q}} f(q)/\rho_F$.[21] With our simplifications one gets

$$P = [\chi q_0^2/(e^2\rho_F)]\mathscr{A}/d .$$

From Eq. (4.3) one finds for r_0 the transcendental equation

$$1 = \mathscr{A} F_d(1/(q_0 r_0)) . \tag{4.11}$$

For large $\mathscr{A}$ this results in a vanishing localization length

$$(q_0 r_0)^2 = d/[A(d-2)], \quad A \gg 1 . \tag{4.12}$$

This formula is equivalent to $P^{-1} = 1 - d^2/[(d+2)\mathscr{A}]$. Hence at the band edges r_0 and χ vanish, while P approaches unity, the signature of perfect localization (see Fig. 1). Approaching the critical point, the localization length diverges. So there is a polarization catastrophe, as discussed in subsection B, and shown in Fig. 1 for $d=3$. Our original predictions concerning this phenomenon[11,24,22] have been reexamined recently[30] in connection with some experimental data.[31] If the whole band is localized, the polarizability reaches its maximum at the band center, as shown in Fig. 1 for $d=3$ and 2.

It was already mentioned that the scaling laws are modified by logarithmic corrections in $d=4$.[22] Equation (4.11) reads, for $d=4$,

$$(A-1)/A = \ln(1+r_0^2 q_0^2)/(r_0 q_0)^2 ,$$

so near the edge one finds, as leading divergency,

$$(r_0 q_0)^2 = (-1/\tau)\ln\tau, \quad \tau \to +0, \quad d=4 . \tag{4.13}$$

The critical exponent for the participation ratio is found here to be the same as the one for χ. This result agrees in leading order with Wegner's $d-2$ expansion.[26,32] Wegner's next-leading term implies the critical exponents for χ and P^{-1} to be different from one another. This result is not reproduced by the present theory, presumably because of our neglecting the CRK's q dependence.

E. Dynamical conductivity for $d=3$

To get the complete dynamical conductivity, one has to solve Eq. (4.3) numerically. This can be done easily by a straightforward iteration procedure. Results for $\sigma(\omega)$ for the conductor phase $A<1$, for the critical point $A=1$, and for the insulating phase $A>1$, are shown in Fig. 2. The low-frequency-current spectrum can be worked out analytically. Using ω as small expansion parameter in Eq. (4.3), one gets, for the conductor phase,

$$\sigma(\omega) = \sigma\left[1 + \frac{\pi}{2\sqrt{2}} A\,|\tau|^{-1} e\left[\frac{\omega\rho_F}{q_0^2\alpha}\right]^{1/2}\right], \quad \omega < \frac{q_0^2\sigma}{\rho_F e^2} \tag{4.14}$$

for the critical point,

$$\sigma(\omega) = \sigma_0 \frac{\sqrt{3}}{2}\left[\frac{\pi}{2}\right]^{2/3}\left[\frac{\omega\rho_F e^2}{q_0^2\sigma_0}\right]^{1/3}, \quad \omega < \frac{q_0^2\sigma_0}{\rho_F e^2} \tag{4.15}$$

and for the insulating phase,

$$\sigma(\omega) = \sigma_0 2 r_0 q_0 [(-A)F'(1/(r_0 q_0))]^{-1}(\omega/\omega^*)^2, \quad \omega < \omega^*\tau \tag{4.16a}$$

$$\omega^* = \sigma_0/(r_0^2\rho_F e^2) . \tag{4.16b}$$

These asymptotes are shown in Fig. 2 as dashed lines.

It is well known from the dynamics of the classical Lorentz problem, that for large times backward scattering dominates so strongly that there is a long-time tail for the velocity autocorrelation function, which is the Fourier

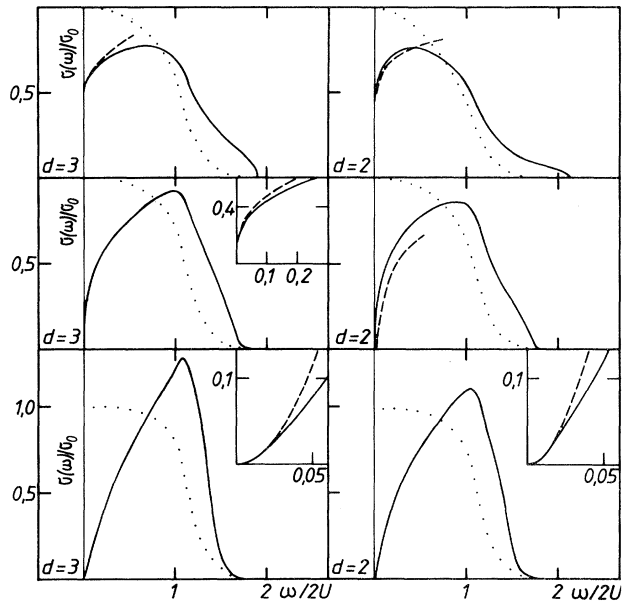

FIG. 2. Normalized dynamical conductivity $\sigma(\omega)$ (solid curves) and lowest-order conductivity $\sigma_0(\omega)$ (dotted curves) vs frequency for $d=2$ and 3 at band center for $n=1$ and $q_0 a=2\pi$. Parameters were chosen as follows (top to bottom): $d=3$—$\mathscr{A}=0.51,1.00;2.70$; $d=2$—$\mathscr{A}=0.19,0.46,1.00$. Dashed curves represent the various scaling laws (see text).

transform of $K''(\omega)$: $K(t)\sim -1/t^{(d+2)/2}$.[33] This implies a nonanalytical low-frequency spectrum $K''(\omega)-K''(0)\sim|\omega|^{d/2}$. Interference enhances this echo in the quantum-mechanical case so strongly, that $K(t)\sim -t^{d/2}$ and $K''(\omega)-K''(0)\sim|\omega|^{(d-2)/2}$, as was first shown for weak coupling within the Edwards model.[16] Equation (4.14) formulates this interference relaxation singularity for the present model and extends the result approximately to all coupling.

At the critical point, one gets a singular rise of the spectrum as already discussed in subsection B. It implies a long-time tail $K(t)\sim -1/t^{4/3}$. In the insulating phase, the correlation function $K(t)$ decreases faster than any power. The spectrum is proportional to ω^2, as predicted by Mott.[34] Actually, there should be a logarithmic correction term due to level repulsion effects, $\sigma(\omega)\sim\omega^2(\ln\omega)^4$,[34,35] which got lost in our approximations.

Notice that the prefactors in Eqs. (4.14) and (4.16a) diverge if the transition point is approached. Simultaneously, however, the ranges of validity of these asymptotic formulas shrink towards zero. These properties reflect the scaling behavior.[26] Another critical phenomenon is the crossover from the hydrodynamic asymptotes, Eqs. (4.14) or (4.16a), for $\hat{\omega}\ll|\tau|^3$, to the critical spectrum, Eq. (4.15), for $\hat{\omega}\gg|\tau|^3$. This is observed, provided one is close enough to the transition point. A corresponding crossover occurs for the long-time tail of $K(t)$. For the interference relaxation the crossover was discussed before within the Edwards model.[25,22] Unfortunately, there are no experiments available to check these predictions for the Anderson transition. It might therefore be worthwhile to mention that the critical dynamics and the mentioned crossover phenomenon was discussed in comparison with molecular-dynamics data for the classical Lorentz problem.[24,36]

F. Quasitransition in $d=2$

It was noticed in subsection B that dimensionality $d=2$ is marginal. So there is no truly metallic state for $d=2$.[8] Equations (4.11) and (4.6) yield a finite localization length r_0 and a finite static polarizability χ in the whole parameter range,

$$(r_0 q_0)^2=\chi q_0^2/(e^2\rho_F)=e^{2/\mathscr{A}}-1\ . \tag{4.17}$$

Close to the band edges perfect localization is observed: The participation ratio approaches unity, as discussed in connection with Eq. (4.12). χ reaches its maximum in the band center. If $\mathscr{A}$ at the band center is not too small compared to unity, the susceptibility, as well as the current spectrum for $d=2$, look rather similar to the results for $d=3$, see Fig. 1 and the third row of Fig. 2.

Even though there is no Anderson transition in a strict sense for $d=2$, there is a critical region in the sense of subsection B. This region is characterized explicitly by $\omega\nu$ and $\mathscr{A}\ll 1$. The self-consistency equation then simplifies to

$$\frac{K(\omega)}{i\alpha_F/\nu}=1+(\mathscr{A}/2)\ln\frac{\omega\rho_F}{q_0^2 K(\omega)}\ . \tag{4.18}$$

For small frequencies this leads to the expected insulator current correlation function:

$$K(\omega)=r_0^2\rho_F[\omega+i\omega^2 r_0^2 2\nu\rho_F/(\mathscr{A}\alpha_F)+\cdots],\quad \omega<\omega^*\ , \tag{4.19}$$

where the localization length is given by the small-$\mathscr{A}$ asymptote of Eq. (4.17): $r_0^2\sim\exp(2/\mathscr{A})$.[23] For larger ω one finds

$$K(\omega)=i(\alpha_F/\nu)\{1+(\mathscr{A}/2)\ln[-i(\omega/\omega^*)/(r_0 q_0)^2]\}\ ,\quad \omega>\omega^*\ . \tag{4.20}$$

The dashed lines in the two upper-right graphs of Fig. 2 represent the formula (4.20). The logarithmic correction term is the critical contribution to the current spectrum due to the interference relaxation. It was first obtained for the Edwards model,[16] and then discussed within the SCCR theory.[22] The crossover frequency ω^*, where the hydrodynamic ω^2 spectrum merges with the interference contribution, is given in Eq. (4.16b).

Let us now choose parameters such that $\mathscr{A}\ll 1$ at the band center. Then there appears the possibility for a quasiphase transition in the following sense. Increasing ϵ_F from the band edge towards the band center yields an increasing localization length, Eq. (4.17). As in the case $d=3$, r_0 is of order $1/q_0$ as long as $\mathscr{A}>1$. At some value $\epsilon_F=\tilde{\epsilon}_c$, $\mathscr{A}$ will decrease below unity, from this point on r_0 and χ will rise rapidly. For energies ϵ_F, which would lead to extended states in $d=3$, r_0 now becomes very large. Similarly, at $\tilde{\epsilon}_c$, P^{-1} will become exceedingly small, as shown in Fig. 1. If ϵ_F crosses $\tilde{\epsilon}_c$, the crossover frequency ω^*, Eq. (4.16b), will become very small, and

$1/\omega^*$ may soon reach macroscopic times. In an experiment, there will be a limited frequency resolution due to, e.g., inelastic scattering processes. If ω^* is smaller than this scattering rate $1/\tau_{in}$, one cannot detect true insulating behavior anymore: $\bar{\sigma}=\sigma(\omega=1/\tau_{in})$ also exhibits a quasitransition at $\tilde{\epsilon}_c$ (Fig. 1). The dynamical spectrum for $\epsilon_F > \tilde{\epsilon}_c$ looks similar to the result for $d=3$, if frequencies are measured on the natural scale $2U$, Fig. 2. The critical spectrum, Eq. (4.20), appears as a strong long-time anomaly.

In this last section we have demonstrated how the quasiphase transition in two-dimensional systems comes about. Since the quasitransition is not accompanied by a mathematical singularity, the transition point $\tilde{\epsilon}_c$ is not well defined. Nevertheless, it should be hard to distinguish from a real phase transition in either real or computer experiment. However, since the present model lacks a genuine weak-coupling limit, the properties of the quasimetallic phase are not as extreme as in the Edwards model.[22]

Note added in proof. After the present work was submitted, H. Mueller and P. Thomas [Phys. Rev. Lett. 51, 702 (1983)] proposed a theory for transport near a mobility edge using methods seemingly similar to ours. Contrary to their claims, however, the third major approximation of these authors is not a mode coupling, but rather a replacement of a vertex vanishing for zero wave vector proportional to k^2 by a k-independent arbitrary function. Consequently, in the limit of static disorder their results disagree with those well known from the literature (cf. our Refs. 8, 16, 22, and 26).

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