

Self-consistent mode-coupling theory of quantum percolation

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We present a novel treatment of the quantum percolation problem that yields a hierarchy of self-consistent equations for the frequency-dependent diffusion coefficient. The first member of this hierarchy is derived and analyzed. This equation predicts that excitations are localized in the presence of any disorder in one and two dimensions, but that a transition from localized to extended excitations takes place for a disordered three-dimensional system. The predicted critical behavior is identical to that obtained by Vollhardt and Wölfle for a Fermi gas in a random potential. The frequency dependence of the ac conductivity and the critical exponents determined from the self-consistent equation agree with the predictions of the scaling theory of Anderson localization.

I. INTRODUCTION

The motion of electrons and other quantum excitations in disordered media has been treated both with completely quantum-mechanical models¹⁻⁶ and with incoherent hopping models that are based on a Pauli master equation.⁷⁻¹⁷ In the quantum treatments, the character of the transport is determined by the degree to which the wave function can be considered to be localized or extended.¹ In the incoherent models, quantum-mechanical phase relationships and tunneling processes are assumed not to play an important role in determining the transport. A fundamental problem in the dynamics of disordered systems is to understand the extent to which purely quantum-mechanical effects, such as phase relationships, are required to explain the motion of excitations. The model of quantum percolation, in which a quantum-mechanical entity propagates through a lattice in which a certain fraction of sites or bonds have been blocked, can provide considerable insight into the role of quantum effects in excitation motion in disordered media.¹⁸⁻²¹ Quantum percolation is a special case of a general class of models that are expected to display quantum localization.¹⁻⁶ Therefore, the conclusions of the scaling theory of quantum localization should apply.^{4,6} The scaling theory predicts that electrons in two dimensions are always localized in the presence of disorder, and hence, that the dc conductivity must vanish. This behavior is to be contrasted with the critical dynamics in an incoherent hopping model, in which a random walker, whose motion is described by a master equation, moves on a disordered lattice, in which a fraction of the sites or bonds have been blocked. For such a model, a metal-insulator transition will occur at the critical concentration for the corresponding, static, site, or bond percolation problem. It is well known that a static percolation transition occurs in two dimensions.²²⁻²⁵ The fact that a metal-insulator transition is expected to be a feature of the incoherent hopping problem in two dimensions, but not of its quantum analog, indicates that study of quantum percolation should provide great insight into the role of quantum effects in electron motion in disordered systems.

In this work, we present a procedure that leads to a hierarchy of self-consistent equations for the diffusion kernel in the quantum percolation problem, evaluated at small frequencies and wave vectors. The behavior of the diffusion kernel in this limit determines the transport properties of this system for long times, and hence, the critical dynamics. The two important dynamical quantities in our approach are the diffusion kernel $D(\mathbf{k}, \epsilon)$ [see Eq. (8)] and $\mathcal{P}_0(t)$, the probability that an excitation that occupies a particular lattice site at time τ can be found at that site at a later time $t + \tau$. We begin with an exact relation between $P_0(\epsilon)$, the Laplace transform of $\mathcal{P}_0(t)$, and $D(\mathbf{k}, \epsilon)$ [Eq. (9)]. We then develop a hierarchy of approximations to the diffusion kernel, in which D is expressed as a functional of $P_0(\epsilon)$, resulting in a second (approximate) relation between these quantities. When the second relation is substituted into the first, we obtain a closed self-consistent equation for D . This equation contains an integration over the wave vector that is conjugate to the position variable. This type of equation is characteristic of mode-coupling theories of nonlinear hydrodynamics, in which self-consistent equations that contain similar integrations over a wave vector are derived.²⁶⁻²⁸ We derive and analyze the first member of this hierarchy of self-consistent equations for the diffusion kernel. This equation predicts that quantum excitations are localized in the presence of any disorder in one and two dimensions, but that a metal-insulator transition from localized to extended excitations occurs for the disordered system in three dimensions. The critical exponents that we obtain are in agreement with the predictions of the scaling theories of Anderson localization.²⁹⁻³³ The critical dynamics predicted by our self-consistent equation for D [Eq. (24)], are identical to those of the equation of Vollhardt and Wölfle.^{34,35} The latter equation was derived for a different model of quantum localization, using very different methods from those employed here. Vollhardt and Wölfle considered a noninteracting Fermi gas at zero temperature in a random potential and obtained their equation by diagrammatic methods. The similarity of the two self-consistent equations suggests that the critical dynamics in these two different models of quantum localization may be related.

II. DERIVATION OF THE SELF-CONSISTENT EQUATION

We consider a lattice in d dimensions with a fraction c of the sites occupied by randomly distributed active particles. The excitation can move among the active particles. The rest of the sites are inaccessible to the excitation. For a given configuration of this random system, the density matrix ρ obeys the Liouville equation

$$\frac{d\rho}{dt} = -iL\rho, \quad (1)$$

$$L = L_0 - i\Lambda. \quad (1a)$$

L_0 is defined by

$$L_0\rho = \hbar^{-1}[H, \rho]. \quad (2)$$

H is the tight-binding Hamiltonian given by

$$H = \hbar \sum_{\substack{i,j \\ (i < j)}} J_{ij} (|i\rangle\langle j| + |j\rangle\langle i|). \quad (3)$$

$|j\rangle$ denotes a state in which the excitation resides on particle j , and J_{ij} is the transfer matrix element between particles i and j . The indices i and j in Eq. (3) label the active particles. In the quantum percolation model, J_{ij} has the value J if particles i and j are nearest neighbors on the lattice, and it is zero otherwise. Λ is a tetradic operator, whose action on ρ is defined by

$$(\Lambda\rho)_{nm} = \sum_{i,j} \Lambda_{nm,ij} \rho_{ij}, \quad (4)$$

$$\Lambda_{nm,ij} = \Gamma \delta_{ni} \delta_{mj} (1 - \delta_{nm}). \quad (5)$$

The effect of Λ is to cause interparticle coherences (e.g., ρ_{ij} , $i \neq j$) to decay with a rate Γ . Λ incorporates the effects of processes that cause coherences to decay but do not affect the dynamics of populations (e.g., ρ_{jj}). Such “pure dephasing” processes can arise, for example, from excited-state phonon interactions. By including Λ in Eq. (1), we adopt a model in which quantum coherences must eventually decay, as they must in any physical system. The effect of the pure dephasing rate Γ on the critical dynamics of the model will be discussed subsequently.

$\mathcal{P}(\mathbf{r}, t)$, the ensemble-averaged probability that an excitation undergoes a displacement \mathbf{r} during a time t , is given by

$$\begin{aligned} \mathcal{P}(\mathbf{r}, t) = & (N-1) \langle [\exp(-iLt)]_{22,11} \delta_{\mathbf{r}, \mathbf{r}_{12}} \rangle \\ & + \delta_{\mathbf{r}, 0} \langle [\exp(-iLt)]_{11,11} \rangle. \end{aligned} \quad (6)$$

The angular brackets in Eq. (6) denote a configuration average. N is the number of active particles. L is the Liouville operator, which is defined in Eq. (2). In the tetradic notation of Eq. (6),³⁶ $[\exp(-iLt)]_{nn,mm}$ is the conditional probability that an excitation propagates from a particle at position \mathbf{r}_m to a particle at position \mathbf{r}_n in time t . $\mathbf{r}_{12} \equiv \mathbf{r}_1 - \mathbf{r}_2$. $P(\mathbf{k}, \varepsilon)$, the Fourier-Laplace transform of $\mathcal{P}(\mathbf{r}, t)$, is defined by

$$P(\mathbf{k}, \varepsilon) = \sum_{\mathbf{r}} \exp(i\mathbf{k} \cdot \mathbf{r}) \int_0^\infty dt \exp(-\varepsilon t) \mathcal{P}(\mathbf{r}, t). \quad (7)$$

$D(\mathbf{k}, \varepsilon)$, the diffusion kernel, is defined by

$$P(\mathbf{k}, \varepsilon) = [\varepsilon + k^2 D(\mathbf{k}, \varepsilon)]^{-1}. \quad (8)$$

If $D(\mathbf{k}, \varepsilon)$ approaches a limit $D(0,0)$ as $k \rightarrow 0$ and $\varepsilon \rightarrow 0$, then for small k and ε , $P(\mathbf{k}, \varepsilon)$ approaches the Green's function of an ordinary diffusion equation with diffusion constant $D(0,0)$. $\mathcal{P}_0(t)$ is defined to be the probability that an excitation that resides at a particular site at time τ will be located at that site at time $t + \tau$. [$\mathcal{P}_0(t) \equiv \mathcal{P}(\mathbf{r}=0, t)$.] $P_0(\varepsilon)$, the Laplace transform of $\mathcal{P}_0(t)$, is related to the diffusion kernel by

$$P_0(\varepsilon) = \Omega^{-1} \int d\mathbf{k} [\varepsilon + k^2 D(\mathbf{k}, \varepsilon)]^{-1}. \quad (9)$$

The integration in Eq. (9) is carried out over the first Brillouin zone, whose “volume” is Ω . [$\Omega = (2\pi)^d / \Omega_0$, where Ω_0 is the volume of the unit cell.]

Equation (9) provides an exact relation between $P_0(\varepsilon)$ and $D(\mathbf{k}, \varepsilon)$. In order to obtain a closed self-consistent equation, we need another independent relation between these two quantities. To that end, we introduce the ansatz

$$D(\mathbf{k}, \varepsilon) \equiv \tilde{D}(\mathbf{k}, P_0(\varepsilon)). \quad (10)$$

According to this ansatz, D is expressed as a functional of P_0 , which depends implicitly on ε through the ε dependence of P_0 . In Appendix A, we expand \tilde{D} in a power series in c :

$$\tilde{D}(\mathbf{k}, P_0) = \sum_{j=1}^{\infty} c^j \tilde{D}_j(\mathbf{k}, P_0). \quad (11)$$

The expansion of \tilde{D} in Eq. (11) should be understood as follows. \tilde{D} depends on c explicitly, in addition to depending implicitly on c through the dependence of P_0 on c . Equation (11) is an expansion of \tilde{D} , with respect to its *explicit* dependence on c . The coefficients \tilde{D}_j depend on c only through the dependence on c of P_0 . Each term in the expansion depends on c to infinite order. Equations (10) and (11) can, therefore, be regarded as a partially resummed density expansion of $D(\mathbf{k}, \varepsilon)$. In Appendix A, we present a procedure by which \tilde{D}_n can be uniquely determined from the coefficients of c^m with $m \leq n$ in the ordinary density expansions of D and P_0 [Eqs. (A2) and (A3)]. The coefficients of c^m in the expansions of D and P_0 can be obtained from the exact values of these quantities for systems with j active particles, where $j \leq m + 1$. The determination of these coefficients is discussed in Appendix B. The expansion in Eq. (11) can be truncated to obtain an approximation $\tilde{D}^{(n)}$ that is exact to order n in c ,

$$\tilde{D}^{(n)}(\mathbf{k}, P_0) = \sum_{j=1}^n c^j \tilde{D}_j(\mathbf{k}, P_0). \quad (12)$$

A hierarchy of self-consistent equations can be constructed according to the following procedure. $\tilde{D}^{(n)}(\mathbf{k}, P_0)$ is substituted for $\tilde{D}(\mathbf{k}, P_0)$ in the right-hand side of Eq. (10). The right-hand side of Eq. (9) is substituted for $P_0(\varepsilon)$ in $\tilde{D}^{(n)}(\mathbf{k}, P_0)$. The result is a closed equation for D .

The purpose of this work is the investigation of the critical dynamics, and hence, the long-time behavior of the present model. At this point, we will restrict our at-

tention to the behavior of D for small ε , which will determine the dynamics at long times. By focusing our attention on the small ε limit of D , we can improve upon approximations to $\tilde{D}(\mathbf{k}, P_0)$ of the form given in Eq. (12). At $c=1$ (no disorder), the model of Eqs. (1)–(5) reduces to the stochastic model of Haken and Strobl for excitation transfer on an ordered lattice.³⁷ $D(\mathbf{k}, \varepsilon)$ can be calculated exactly for this model, although its form for arbitrary values of ε is rather complicated.³⁸ In the $\varepsilon \rightarrow 0$ limit, however, $D(\mathbf{k}, \varepsilon)$ becomes independent of ε and takes the following form for the d -dimensional generalization of a simple cubic lattice:

$$\bar{D} = k^{-2}(4J^2/\Gamma) \left[d - \sum_{j=1}^d \cos(\mathbf{k} \cdot \mathbf{a}_j) \right]. \quad (13)$$

In Eq. (13) we have denoted D at $c=1$ by \bar{D} . \mathbf{a}_j is the lattice vector in the j th direction. We now have two pieces of information regarding \tilde{D} : a truncated expansion in c [Eq. (12)] that will be accurate for $c < 1$, and the exact form in the $\varepsilon \rightarrow 0$ limit at $c=1$ [Eq. (13)]. By constructing an approximation to \tilde{D} that interpolates between Eqs. (12) and (13), we guarantee that the self-consistent equation will give exact results at $c=1$ in the $\varepsilon \rightarrow 0$ limit. A hierarchy of such approximations can be derived by constructing Padé approximants in the variable $\gamma \equiv c/(1-c)$:

$$\tilde{D}(\mathbf{k}, P_0) = \left[\sum_{m=1}^j a_m \gamma^m \right] / \left[1 + \sum_{m=1}^j b_m \gamma^m \right]. \quad (14)$$

The coefficients a_m and b_m in Eq. (14) are obtained by requiring that Eq. (14) reduce to Eq. (12) in the limit $c \rightarrow 0$ and to Eq. (13) at $c=1$.

We shall derive the self-consistent equation for D that is based on the first member of this hierarchy. Setting $j=1$ in Eq. (14) yields

$$\tilde{D}(\mathbf{k}, P_0) = \gamma \tilde{D}_1(\mathbf{k}, P_0) / [1 + \gamma \tilde{D}_1(\mathbf{k}, P_0) / \bar{D}]. \quad (15)$$

In Appendix A [Eq. (A8)], we show that $\tilde{D}_1(\mathbf{k}, P_0)$ can be obtained by calculating $D_1(\mathbf{k}, \varepsilon^{-1})$, the first term in the density expansion of $D(\mathbf{k}, \varepsilon)$, and replacing ε^{-1} with P_0 . The calculation of $D_1(\mathbf{k}, \varepsilon^{-1})$ from the exact solution of the two-particle problem is outlined in Appendix B. The result is

$$k^2 D_1(\mathbf{k}, \varepsilon^{-1}) = \{4J^2 \varepsilon / [\varepsilon(\varepsilon + \Gamma) + 4J^2]\} \left[d - \sum_{j=1}^d \cos q_j \right], \quad (16)$$

$$q_j = \mathbf{k} \cdot \mathbf{a}_j. \quad (17)$$

In the small ε limit ($\varepsilon \ll \Gamma$), we replace the denominator of the first factor on the right-hand side of Eq. (16) with $\varepsilon \Gamma + 4J^2$. Application of Eq. (A8) yields

$$k^2 \tilde{D}_1(\mathbf{k}, P_0) = [4J^2 / (\Gamma + 4J^2 P_0)] \left[d - \sum_{j=1}^d \cos q_j \right]. \quad (18)$$

Substitution of Eqs. (13) and (18) into Eq. (15) yields our final expression for \tilde{D} :

$$k^2 \tilde{D}(\mathbf{k}, P_0) = \{2ca^{-2} D_0 / [1 + 2(1-c)a^{-2} D_0 P_0]\} \times \left[d - \sum_{j=1}^d \cos q_j \right], \quad (19)$$

$$D_0 \equiv 2J^2 a^2 / \Gamma. \quad (20)$$

In Eqs. (19) and (20), a is the lattice constant. We will focus on the long-wavelength (small k) dynamics by taking the $k \rightarrow 0$ limit of Eq. (19):

$$\begin{aligned} D(\varepsilon) &\equiv \lim_{k \rightarrow 0} D(\mathbf{k}, \varepsilon) \\ &= \lim_{k \rightarrow 0} \tilde{D}(\mathbf{k}, P_0) \\ &= c D_0 / [1 + 2(1-c)a^{-2} D_0 P_0]. \end{aligned} \quad (21)$$

To obtain a closed equation for $D(\varepsilon)$, we rewrite Eq. (9) in terms of $D(\varepsilon)$,

$$P_0(\varepsilon) = [a^2 / 2D(\varepsilon)] I_d(a^2 \varepsilon / 2D(\varepsilon)). \quad (22)$$

$I_d(x)$, which is the diagonal element of the Green's function for the d -dimensional analog of a simple-cubic lattice,^{39–41} is given by

$$I_d(x) = \pi^{-d} \int_0^\pi dq_1 \cdots \int_0^\pi dq_d \left[x + d - \sum_{j=1}^d \cos q_j \right]^{-1}. \quad (23)$$

Substituting Eq. (22) into the denominator of Eq. (21) yields a self-consistent equation for $D(\varepsilon)$, the $k \rightarrow 0$ limit of the diffusion kernel,

$$D(\varepsilon) / D_0 = c - (1-c) I_d(\varepsilon a^2 / 2D(\varepsilon)). \quad (24)$$

Equation (24) is the primary result of this work, and will be analyzed in the following section.

III. RESULTS AND DISCUSSION

In this section, we analyze Eq. (24), the self-consistent equation for the diffusion kernel in the limit of small frequencies and wave vectors. The behavior of this equation in d dimensions depends on the properties of $I_d(x)$, which is defined in Eq. (23). $I_d(x)$ is the diagonal element of the lattice Green's function for the d -dimensional analog of the simple-cubic lattice.^{39–41} The analytic properties of these functions are well known.^{39–41} The argument of I_d in Eq. (24) is $a^2 \varepsilon / 2D$. For $c > c^*$, the critical concentration for quantum percolation, we expect that $D(\varepsilon)$ will approach a finite limit as $\varepsilon \rightarrow 0$, and hence, that $a^2 \varepsilon / D$ becomes arbitrarily small for sufficiently small ε . For $c < c^*$, we expect $D(\varepsilon) \sim A \varepsilon$ as $\varepsilon \rightarrow 0$, where A is a function of c that diverges as c approaches c^* from below. As $\varepsilon \rightarrow 0$, $a^2 \varepsilon / D$ will approach the limit $a^2 A^{-1}$, which goes to zero as c approaches c^* . Thus, in evaluating Eq. (24) in the vicinity of a critical point ($c > c^*$ and $c < c^*$), we need only consider the behavior of $I_d(x)$ for small values of x . The limiting behavior of $I_d(x)$ in one, two, and three dimensions is^{39–41}

$$\lim_{x \rightarrow 0} I_d(x) = \begin{cases} (2x)^{-1/2}, & d=1 \\ (2\pi)^{-1} \ln(x^{-1}), & d=2 \\ I_3(0) - \pi^{-1}(x/2)^{1/2}, & d=3 \end{cases} \quad (25)$$

with

$$I_3(0) \approx 0.5055. \quad (25a)$$

By substituting the three expressions in Eq. (25) into Eq. (24), we obtain self-consistent equations for $D(\epsilon)$ that are valid for small ϵ in the vicinity of the critical point. We shall now analyze the resulting equation in one, two, and three dimensions. In one dimension ($d=1$), the equation assumes the form

$$D(\epsilon)/D_0 = c - (1-c)[D(\epsilon)/a^2\epsilon]^{1/2}. \quad (26)$$

In the $\epsilon \rightarrow 0$ limit, the physically reasonable solution of this quadratic equation for $D^{1/2}$ assumes the form

$$D(\epsilon) = \begin{cases} [c/(1-c)]^2 a^2 \epsilon, & c < 1 \\ D_0, & c = 1. \end{cases} \quad (27)$$

At $c=1$, Eq. (26) yields $D(\epsilon) = D_0$, which is the exact result. The form of our approximation to $\tilde{D}(\mathbf{k}, P_0)$ in Eqs. (14) and (15) guarantees that Eq. (24) will be exact at $c=1$. Equation (27) shows that for $d=1$ the diffusion kernel vanishes as $\epsilon \rightarrow 0$ for all $c < 1$. The percolation transition occurs at $c^* = 1$, which is the correct result. For $d=2$, substitution of Eq. (25) into Eq. (24) yields

$$D(\epsilon)/D_0 = c - [(1-c)/2\pi] \ln[2D(\epsilon)/a^2\epsilon]. \quad (28)$$

If we try a solution of the form $D(\epsilon) = A\epsilon^\alpha$ as $\epsilon \rightarrow 0$, we can see by direct substitution in Eq. (28), that $\alpha=1$ for all $c < 1$, and that $\alpha=0$ at $c=1$. The solution of Eq. (28) for small ϵ assumes the form

$$D(\epsilon) = \begin{cases} \exp[2\pi c/(1-c)](a^2\epsilon/2), & c < 1 \\ D_0, & c = 1. \end{cases} \quad (29)$$

As in the case of $d=1$, $D(\epsilon) = A\epsilon$ as $\epsilon \rightarrow 0$ for all $c < 1$, where A is function of c that diverges as $c^* = 1$ is approached. Thus, Eq. (24) predicts a quantum percolation transition at $c=1$ in two dimensions. This result agrees with the predictions of the scaling theory of quantum localization, according to which a quantum excitation is always localized in two dimensions in the presence of any finite amount of disorder.⁶ This prediction is to be contrasted with the well-known results for the classical site and bond percolation problems, in which a transition occurs at $c^* < 1$ for two-dimensional lattices.²²⁻²⁵

Substitution of Eq. (25) into Eq. (24) yields the following self-consistent equation for $d=3$:

$$D(\epsilon)/D_0 = c - (1-c)\{I_3(0) - (2\pi)^{-1}[\epsilon a^2/D(\epsilon)]^{1/2}\}. \quad (30)$$

Equation (30) is a cubic equation in $D(\epsilon)$ and it can be recast in the form

$$D(\epsilon)[D(\epsilon)/D_0 - (c - c^*)(1 - c^*)^{-1}]^2 = (a/2\pi)^2(1 - c)^2\epsilon, \quad (31)$$

where

$$c^* = I_3(0)/[1 + I_3(0)] \approx 0.3358. \quad (32)$$

The solution to Eq. (31) can be explored by again making the ansatz $D(\epsilon) = A\epsilon^\alpha$ and checking for consistency. This procedure reveals that $c = c^*$ is a critical point. $\alpha=1$ for $c < c^*$, $\alpha=0$ for $c > c^*$, and $\alpha = \frac{1}{3}$ for $c = c^*$. We then get, for $d=3$

$$D(\epsilon) = \begin{cases} Ba^2(c^* - c)^{-2}\epsilon - 2B^2(a^4/D_0) \\ \quad \times (c^* - c)^{-5}(1 - c^*)\epsilon^2, & c < c^* \\ D_0(1 - c^*)^{-1}(c - c^*), & c > c^* \\ [D_0 a(1 - c^*)/2\pi]^{2/3}\epsilon^{1/3}, & c = c^*, \end{cases} \quad (33a)$$

$$(33b)$$

$$(33c)$$

with

$$B = [(1-c)(1-c^*)/2\pi]^2. \quad (34)$$

Thus, Eq. (30) predicts a transition from localized to extended excitations at $c^* \approx 0.3358$. For $c < c^*$, $D(\epsilon)$ is linear in ϵ for small ϵ , with a coefficient that diverges as $(c^* - c)^{-2\nu}$. For $c > c^*$, $D(\epsilon)$ approaches a constant value for small ϵ that vanishes as $(c - c^*)^s$. The critical exponents predicted by Eq. (30) are $\nu=1$ and $s=1$, which obey the scaling relation $s = (d-2)\nu$, which was derived by Wegner.³⁰ At the critical point ($c = c^*$), $D(\epsilon) \sim \epsilon^{1/3}$. Equations (33) can be used to determine the behavior at long times of $\langle r^2(t) \rangle$, the mean-squared displacement of an excitation. The Laplace transform of $\langle r^2(t) \rangle$ is related to $D(\epsilon)$ by

$$\int_0^\infty dt \exp(-\epsilon t) \langle r^2(t) \rangle = 2d\epsilon^{-2}D(\epsilon). \quad (35)$$

The asymptotic behavior of $\langle r^2(t) \rangle$ can be obtained from Eqs. (33) and (35), using the Tauberian theorem for Laplace transforms.⁴² The result is

$$\lim_{t \rightarrow \infty} \langle r^2(t) \rangle \sim \begin{cases} Ba^2(c^* - c)^{-2}, & c < c^* \\ D_0(1 - c^*)^{-1}(c - c^*)t, & c > c^* \\ [D_0 a(1 - c^*)/2\pi]^{2/3}t^{2/3}, & c = c^*. \end{cases} \quad (36)$$

The ac conductivity is related to $D(\epsilon)$ by^{29,34}

$$\sigma(\omega) \sim \text{Re}D(-i\omega). \quad (37)$$

Equation (33) can therefore be used to predict the behavior of $\sigma(\omega)$ in the vicinity of a metal-insulator transition. For $c > c^*$, we have

$$\sigma(0) \sim D_0(1 - c^*)^{-1}(c - c^*). \quad (38)$$

On the insulating side of the transition ($c < c^*$) $\sigma(\omega)$ will be proportional to ω^2 for small ω ,

$$\sigma(\omega) \sim 2B^2(a^4/D_0)(c^* - c)^{-5}(1 - c^*)\omega^2. \quad (39)$$

At higher frequencies, there is a contribution to $\sigma(\omega)$ that is proportional to $\omega^{1/3}$. This behavior can be obtained from the exact solution to Eq. (31), which is

$$D(\epsilon) = [D_0 a(1 - c)/4\pi]^{2/3}\epsilon^{1/3} \\ \times \{ [1 + (1 + \epsilon_c/\epsilon)^{1/2}]^{1/3} \\ + [1 - (1 + \epsilon_c/\epsilon)^{1/2}]^{1/3} \}^2. \quad (40)$$

The crossover frequency ε_c is given by

$$\varepsilon_c = (16\pi^2/27)(D_0/a^2)(1-c^*)^{-3}(1-c)^{-2}(c^*-c)^3. \quad (41)$$

For $\varepsilon \gg \varepsilon_c$, Eq. (40) shows that $D(\varepsilon)$ is proportional to $\varepsilon^{1/3}$. At $c=c^*$, ε_c vanishes [see Eq. (41)], and this behavior obtains in the limit $\varepsilon \rightarrow 0$, in accordance with Eq. (33c). Substituting $-i\omega$ for ε in Eqs. (40) and (41) shows that, for $\omega \gg \omega_c$,

$$\sigma(\omega) \sim [D_0 a (1-c)/2\pi]^{2/3} \omega^{1/3}. \quad (42)$$

The crossover frequency ω_c , at which the $\omega^{1/3}$ dependence begins to dominate the ω^2 dependence, vanishes as c approaches c^* from below,

$$\omega_c \sim (c^* - c)^3. \quad (43)$$

This frequency dependence of $\sigma(\omega)$ agrees with the predictions of scaling theories.²⁹⁻³³

In defining the present model with Eqs. (1)–(5), we included the relaxation operator Λ in the Liouville equation, whose effect is to cause quantum coherences to decay with the pure dephasing rate Γ . Since quantum percolation models do not usually include such a relaxation operator, it is important to consider the influence of pure dephasing on our final results. Examination of Eqs. (24), (29), and (33) indicates that the $\varepsilon \rightarrow 0$ behavior of $D(\varepsilon)$ for $c < c^*$ in any dimension is unaffected by the presence of pure dephasing. The pure dephasing rate Γ is contained in $D_0 \equiv 2J^2 a^2 / \Gamma$, which does not appear in the expressions for $D(\varepsilon)$ for $c < c^*$ and $\varepsilon \rightarrow 0$ [Eqs. (27), (29), and (33a)]. [The correction of order ε^2 in Eq. (33a) does depend on Γ .] For $c > c^*$ in $d=3$, D approaches a constant value as $\varepsilon \rightarrow 0$, which is proportional to D_0 . If pure dephasing processes had not been included, our self-consistent equation [Eq. (24)] would not have a solution in $d=3$ for which $D(\varepsilon)$ approaches a constant as $\varepsilon \rightarrow 0$ for $c > c^*$. Such a solution does exist, however, for arbitrarily small values of the pure dephasing rate Γ . Whether the addition of a pure dephasing rate of arbitrarily small magnitude is sufficient to qualitatively alter the critical dynamics of the quantum percolation model, is an open question. It is clear, though, that including such relaxation processes is physically reasonable, since quantum coherences must eventually decay in real systems.

The critical exponents, calculated from Eq. (24), are identical to those obtained by Vollhardt and Wölfle (VW) for a different model of quantum localization.^{29,34,35} VW treated a gas of noninteracting fermions at zero temperature in the presence of randomly placed static scatterers. Using a diagrammatic method, they derived the following self-consistent equation for $D(\varepsilon)$:

$$D(\varepsilon)/D_0 = 1 - d\lambda k_F^{2-d} K_d(\varepsilon/D(\varepsilon)), \quad (44)$$

$$K_d(x) = \int_0^{k_0} \frac{k^{d-1} dk}{k^2 + x}. \quad (45)$$

k_F is the Fermi wave vector, k_0 is a cutoff wave vector, and $\lambda = \hbar / (2\pi E_F \tau)$, where E_F is the Fermi energy, and τ is the transport relaxation time of the electrons. For small values of its argument, K_d is given by

$$\lim_{x \rightarrow 0} K_d(x) = \begin{cases} \pi/(2x^{1/2}), & d=1 \\ \frac{1}{2} \ln(k_0^2/x), & d=2 \\ k_0 - (\pi/2)x^{1/2}, & d=3. \end{cases} \quad (46)$$

Comparison of Eqs. (25) and (46) shows that $K_d(x)$, which appears in the VW equation [Eq. (44)] has the same behavior as $x \rightarrow 0$ as $I_d(x)$, which appears in our result [Eq. (24)]. Comparison of Eqs. (24) and (25) to Eqs. (44) and (46) shows that our self-consistent equation is identical in structure to that of VW. In particular, let us compare them for $d=3$. Substitution of Eq. (46) into Eq. (44) yields the VW equation in $d=3$,

$$D(\varepsilon)/D_0 = 1 - 3\lambda k_F^{-1} [k_0 - (\pi/2)(\varepsilon/D)^{1/2}]. \quad (47)$$

Replacing D_0 with cD_0 , λk_F^{-1} with $(a/3\pi^2) [(1-c)/c]$, and k_0 with $\pi^2 I_3(0) a^{-1}$ in Eq. (47) yields Eq. (30), our self-consistent equation for quantum percolation in $d=3$. It should be noted that VW introduce a cutoff wave vector k_0 in their derivation of Eq. (44). The critical value of the disorder parameter λ within their formulation depends on k_0 . In our derivation, we did not have to introduce such a cutoff wave vector, and we have a numerical prediction for c^* [Eq. (32)].

It is remarkable that the same self-consistent equation should be derived for two different models of quantum localization, using very different approaches. The starting point for the VW resummation is a perturbation expansion in scattering events, in which the zeroth-order problem is the *delocalized* Fermi gas. Our resummation procedure is based on an expansion in c , the concentration of conducting sites, and hence, the zeroth-order problem in our treatment of quantum percolation is a *localized* electron. In the VW treatment, the two relevant dynamical quantities are $D(\mathbf{k}, \varepsilon)$, the diffusion kernel, and $M(\mathbf{k}, \varepsilon)$, the current relaxation kernel. In the present treatment, we focus on D and P_0 . However, the types of disorder in the two models are very similar, since the unoccupied sites in the quantum percolation model can be regarded as randomly placed static scatterers. The fact that our treatment of quantum percolation leads to an equation that is identical in structure to the VW equation suggests a connection between the critical dynamics of these two different models.

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APPENDIX A

In this work we have made the ansatz that the diffusion kernel could be expressed as a functional of P_0 ,

$$D(\mathbf{k}, \varepsilon, c) = \tilde{D}(\mathbf{k}, P_0(\varepsilon, c), c). \quad (A1)$$

In this appendix we write P_0 as $P_0(\varepsilon, c)$, D as $D(\mathbf{k}, \varepsilon, c)$, and \tilde{D} as $\tilde{D}(\mathbf{k}, P_0, c)$ to emphasize the dependence of these quantities on concentration. Equation (A1) is a definition of the functional \tilde{D} . In this appendix, we present a systematic prescription for evaluating \tilde{D} . We begin by expanding D and P_0 in powers of c ,

$$D(\mathbf{k}, \varepsilon, c) = \sum_{j=1}^{\infty} c^j D_j(\mathbf{k}, \varepsilon^{-1}), \quad (\text{A2})$$

$$P_0(\varepsilon, c) = \varepsilon^{-1} + \sum_{j=1}^{\infty} c^j Q_j(\varepsilon^{-1}). \quad (\text{A3})$$

D_j and Q_j can be calculated from the exact solution of the transport problem for $j+1$ or fewer particles. We shall take $\{D_j\}$ and $\{Q_j\}$ as given and use them to construct an expression for \tilde{D} . $\tilde{D}(\mathbf{k}, P_0, c)$ depends explicitly on c , as well as depending implicitly on c through the c dependence of P_0 . We expand \tilde{D} in a power series with respect to its explicit c dependence,

$$\tilde{D}(\mathbf{k}, P_0, c) = \sum_{j=1}^{\infty} c^j \tilde{D}_j(\mathbf{k}, P_0). \quad (\text{A4})$$

The function $D_n(\mathbf{k}, \varepsilon^{-1})$ in Eq. (A2) is given by

$$\begin{aligned} D_n(\mathbf{k}, \varepsilon^{-1}) &= \frac{1}{n!} \left. \frac{\partial^n}{\partial c^n} D(\mathbf{k}, \varepsilon, c) \right|_{c=0} \\ &= \frac{1}{n!} \left. \frac{\partial^n}{\partial c^n} \tilde{D}(\mathbf{k}, P_0, c) \right|_{c=0}. \end{aligned} \quad (\text{A5})$$

The second equality in Eq. (A5) follows from the definition of \tilde{D} in Eq. (A1). Substitution of Eq. (A4) into Eq. (A5) and application of Leibnitz's rule for the n th derivative of a product yields

$$D_n(\mathbf{k}, \varepsilon^{-1}) = \sum_{j=1}^n \frac{1}{(n-j)!} \left. \frac{\partial^{n-j}}{\partial c^{n-j}} \tilde{D}_j(\mathbf{k}, P_0) \right|_{c=0}. \quad (\text{A6})$$

An expression for $\tilde{D}_n(\mathbf{k}, P_0)$ is obtained by solving Eq. (A6) for $\tilde{D}_n(\mathbf{k}, \varepsilon^{-1})$ and replacing ε^{-1} with P_0 ,

$$\begin{aligned} \tilde{D}_n(\mathbf{k}, P_0) &= D_n(\mathbf{k}, P_0) - \sum_{j=1}^{n-1} \frac{1}{(n-j)!} \left. \frac{\partial^{n-j}}{\partial c^{n-j}} \right. \\ &\quad \times \tilde{D}_j(\mathbf{k}, P_0(x, c)) \Big|_{c=0, x=P_0}. \end{aligned} \quad (\text{A7})$$

Equation (A7) relates \tilde{D}_n to D_n and to $\{\tilde{D}_j\}$ with $j < n$. Using Eqs. (A2), (A3), and (A7), we can relate the unknown function \tilde{D}_n to the known functions D_j and Q_j with $j \leq n$. In this manner, we may calculate each term in the series for \tilde{D} in Eq. (A4). For illustrative purposes, we will calculate $\tilde{D}_n(\mathbf{k}, P_0)$ explicitly for $n=1$ and $n=2$. For $n=1$, Eq. (A7) becomes

$$\tilde{D}_1(\mathbf{k}, P_0) = D_1(\mathbf{k}, P_0). \quad (\text{A8})$$

For $n=2$, we have

$$\begin{aligned} \tilde{D}_2(\mathbf{k}, P_0) &= D_2(\mathbf{k}, P_0) - \left. \frac{\partial}{\partial c} \tilde{D}_1(\mathbf{k}, P_0(x, c)) \right|_{c=0, x=P_0} \\ &= D_2(\mathbf{k}, P_0) - \left. \frac{\partial \tilde{D}_1(\mathbf{k}, y)}{\partial y} \right|_{y=P_0} \left. \frac{\partial P_0(x, c)}{\partial c} \right|_{c=0, x=P_0} \\ &= D_2(\mathbf{k}, P_0) - Q_1(P_0) \left. \frac{\partial D_1(\mathbf{k}, y)}{\partial y} \right|_{y=P_0}. \end{aligned} \quad (\text{A9})$$

APPENDIX B

In this appendix we outline the derivation of Eq. (16), the first term of the density expansion of the diffusion kernel $D(\mathbf{k}, \varepsilon)$. We begin by considering the propagator $\mathcal{P}^{(N)}(\mathbf{r}, \mathbf{r}', t)$ for a finite lattice of M sites, N of which are occupied by active particles. $\mathcal{P}^{(N)}(\mathbf{r}, \mathbf{r}', t)$ is the configuration-averaged probability that an excitation migrates from a position \mathbf{r}' to a position \mathbf{r} in time t . It is the analog for a finite system of $\mathcal{P}(\mathbf{r}, t)$, defined in Eq. (6). Since a finite lattice is not translationally invariant, $\mathcal{P}^{(N)}$ depends on \mathbf{r} and \mathbf{r}' separately and not just on their difference. $\mathcal{P}^{(N)}$ can be written in the form

$$\begin{aligned} \mathcal{P}^{(N)}(\mathbf{r}, \mathbf{r}', t) &= 1 + \frac{(N-1)}{(M-1)} \mathcal{P}_1^{(M)}(\mathbf{r}, \mathbf{r}', t) \\ &\quad + \frac{(N-1)(N-2)}{(M-1)(M-2)} \mathcal{P}_2^{(M)}(\mathbf{r}, \mathbf{r}', t) + \cdots \end{aligned} \quad (\text{B1})$$

Taking the thermodynamic limit of Eq. (B1) ($N \rightarrow \infty$, $M \rightarrow \infty$, $N/M = c$) yields the density expansion of $\mathcal{P}(\mathbf{r} - \mathbf{r}', t)$:

$$\mathcal{P}(\mathbf{r} - \mathbf{r}', t) = 1 + c \mathcal{P}_1(\mathbf{r} - \mathbf{r}', t) + c^2 \mathcal{P}_2(\mathbf{r} - \mathbf{r}', t) + \cdots, \quad (\text{B2})$$

$$\mathcal{P}_n(\mathbf{r} - \mathbf{r}', t) = \lim_{M \rightarrow \infty} \mathcal{P}_n^{(M)}(\mathbf{r}, \mathbf{r}', t). \quad (\text{B3})$$

For $N=2$, Eq. (B1) becomes

$$\mathcal{P}^{(2)}(\mathbf{r}, \mathbf{r}', t) = 1 + (M-1)^{-1} \mathcal{P}_1^{(M)}(\mathbf{r}, \mathbf{r}', t). \quad (\text{B4})$$

Taking the $M \rightarrow \infty$ limit of Eq. (B4) gives

$$\mathcal{P}_1(\mathbf{r} - \mathbf{r}', t) = \lim_{M \rightarrow \infty} (M-1) [\mathcal{P}^{(2)}(\mathbf{r}, \mathbf{r}', t) - 1]. \quad (\text{B5})$$

$\mathcal{P}^{(2)}(\mathbf{r}, \mathbf{r}', t)$ is the configuration-averaged propagator for two interacting particles with nearest-neighbor interactions on a lattice of M sites. It can be determined exactly

by solving the Liouville equation [Eq. (1)] for two particles and performing a configuration average. The final result for $P_1(\mathbf{k}, \varepsilon)$, the Fourier-Laplace transform of $\mathcal{P}_1(\mathbf{r}, t)$ [see Eq. (7)], is

$$P_1(\mathbf{k}, \varepsilon) = \frac{4J^2/\varepsilon}{\varepsilon(\varepsilon + \Gamma) + 4J^2} \left[\sum_{j=1}^d \cos(\mathbf{k} \cdot \mathbf{a}_j) - d \right]. \quad (\text{B6})$$

\mathbf{a}_j is the lattice vector in the j th direction. $P_1(\mathbf{k}, \varepsilon)$ is the

coefficient of c in a density expansion of $P(\mathbf{k}, \varepsilon)$. $D(\mathbf{k}, \varepsilon)$ is related to $P(\mathbf{k}, \varepsilon)$ by Eq. (8). From this equation, $D_1(\mathbf{k}, \varepsilon^{-1})$, the coefficient of c in a density expansion of $D(\mathbf{k}, \varepsilon)$, is given by

$$k^2 D_1(\mathbf{k}, \varepsilon^{-1}) = -\varepsilon^2 P_1(\mathbf{k}, \varepsilon). \quad (\text{B7})$$

Substitution of Eq. (B6) into Eq. (B7) results in Eq. (16).

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