

Absence of localization in certain statically disordered lattices in any spatial dimension

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(Received 30 May 1989)

We present a statically disordered electronic system in which under certain circumstances an initially localized particle necessarily becomes delocalized at long times regardless of the spatial dimension and the magnitude of the disorder. The model is based on correlations between diagonal and off-diagonal matrix elements and is shown to be applicable to structurally induced disorder in solids. Numerical and analytical calculations in one dimension indicate that transport is superdiffusive, with the mean-square displacement growing in time as $t^{3/2}$, regardless of the magnitude of the disorder. Transport is shown to arise in this model from a set of measure-zero unscattered states at a particular energy in the parent-ordered band. It is argued that, when the Fermi level coincides with the energy of the unscattered states, an enhancement of transport should obtain. In addition, it is shown that superdiffusive motion persists for a wide range of correlations between the diagonal and off-diagonal matrix elements when the disorder is structurally induced and chosen from a bivalued distribution. The relevance of these results to transport experiments is discussed.

I. INTRODUCTION

One of the widely accepted results in solid-state physics is that all the electronic states of a disordered one-dimensional system are exponentially localized, even for infinitesimal values of the disorder.¹⁻⁵ The existence of exponentially localized states is generally believed to lead to an absence of diffusion or long-range transport in such systems. The early work of Anderson on the site-diagonal disorder in tight-binding models,^{1,2} and of Mott and Twose,³ form the basis for the prevalence of this view. Although it is realized,⁴ however, that certain disordered electronic systems might exist in which exponential localization does not obtain, no such model has yet been constructed. Nonetheless, in this paper we present a physically realizable disordered electronic system in which an initially localized particle will necessari-

ly become delocalized at long times, regardless of the spatial dimension and the magnitude of the disorder. We present numerical and analytical calculations in one dimension that indicates that the transport of an initially localized particle is superdiffusive. We show that our results can be explained by the presence of electronic states whose localization lengths diverge.

The model we consider is one in which the site energy ϵ_m , at site m is correlated with the off-diagonal matrix elements $V_{m,n}$. Such a correlation between the disorder-induced fluctuations of the matrix elements of the Hamiltonian may be described with various models, depending upon the source of the disorder. However, we consider specifically, the correlation between ϵ_m and $V_{m,n}$ that arises in the standard⁶ single-particle Hamiltonian in which the particle energy is coupled linearly to the dilation of the lattice

$$H = \sum_m \epsilon_0 a_m^\dagger a_m + \sum_{m,\mu} V_\mu a_m^\dagger a_{m+\hat{\mu}} + V_\mu^* a_{m+\hat{\mu}}^\dagger a_m + \sum_{m,\mu} \gamma_\mu (x_m^\mu - x_{m+\hat{\mu}}^\mu) a_m^\dagger a_{m+\hat{\mu}} + \gamma_\mu^* (x_m^\mu - x_{m+\hat{\mu}}^\mu) a_{m+\hat{\mu}}^\dagger a_m + \sum_{m,\mu} G_\mu [(x_{m+\hat{\mu}}^\mu - x_m^\mu) + (x_m^\mu - x_{m-\hat{\mu}}^\mu)] a_m^\dagger a_m + H_{\text{lattice}}. \quad (1.1)$$

In Eq. (1.1) $\hat{\mu}$ is a unit vector pointing along the μ th direction from the site m to its neighbor along that direction. The electronic operators a_m^\dagger , create an electron at site m with energy ϵ_0 , and x_m^μ is the displacement from equilibrium, in the μ th direction, of the ion at site m . The energy of the bare lattice is denoted by H_{lattice} . We remind the reader that the electron-lattice coupling terms are such that, when the m th ion moves closer to its neighbor at site $m+1$ by an amount

$$\Delta_{m,m+\hat{\mu}}^\mu = (x_m^\mu - x_{m+\hat{\mu}}^\mu),$$

the electronic energy at site m and the transfer-matrix element change linearly by an amount $G_\mu \Delta_{m,m+\hat{\mu}}^\mu$ and $\gamma_\mu \Delta_{m,m+\hat{\mu}}^\mu$, respectively. The linear form of the interactions may arise, for example, from the lowest-order term in a Taylor-series expansion about the equilibrium positions of the ions. Note that we have considered only the dominant nearest-neighbor interactions. This form of electron-lattice coupling is often taken to describe structurally induced disorder in solids. For example, Su, Schrieffer, and Heeger⁷ have considered this model with off-diagonal coupling only in the context of transport in

perfectly dimerized polyacetylene. The electron-phonon coupling constants G_μ and γ_μ represent the first-order terms in a Taylor-series expansion (in the displacement of the ions) of the diagonal and the off-diagonal matrix elements in the electronic basis, respectively. In the general case, the off-diagonal matrix elements may be complex. For simplicity, we will choose V_μ and γ_μ to be of the form $V_\mu e^{i\phi_\mu}$ and $\gamma_\mu e^{i\theta_\mu}$, where the complex nature is entirely contained in the phase angles ϕ_μ and θ_μ . It is instructive at this time to point out the profound effect correlations between site and off-diagonal disorder have on the eigenstates of H . To see this, we write Eq. (1.1) in momentum space:

$$H = H_{\text{lattice}} + \sum_{\mathbf{k}} \varepsilon_0 a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + \sum_{\mathbf{k}, \mu} 2V_\mu \cos(\phi_\mu - k_\mu) a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + \sum_{\mathbf{k}, \mathbf{q}, \mu} 2i[\gamma_\mu \sin(k_\mu - \theta_\mu) - \gamma_\mu \sin(k_\mu - q_\mu - \theta_\mu) - G_\mu \sin(q_\mu)] x_{\mathbf{q}}^\mu a_{\mathbf{k}}^\dagger a_{\mathbf{k} - \hat{\mu} q_\mu}, \quad (1.2)$$

where $a_{\mathbf{k}}^\dagger$ creates an electron with dimensionless crystal-momentum \mathbf{k} , and $x_{\mathbf{q}}^\mu$ is the discrete Fourier transform of x_m^μ . The last term in Eq. (1.2) contains the effects of the dynamic electron-phonon coupling. We see directly from (1.2) that the magnitude of this term, which modulates the scattering of the electron, is governed entirely by the coupling constants G_μ and γ_μ . In fact, for the special case when $\gamma_\mu = G_\mu$, the scattering term disappears altogether for $\mathbf{k}_\mu = \theta_\mu$ for each μ . Hence, there is an absence of scattering of a particular electronic state when G_μ is equal to γ_μ , regardless of their magnitude and the spatial dimension of the system. The absence of scattering is a direct consequence of correlations between the site-

diagonal and site-off-diagonal matrix elements. The particular electronic state that remains unscattered possesses a wave vector $k = \{\theta_1, \theta_2, \theta_3, \dots, \theta_d\}$ in the parent-ordered band.

This result is true whether the disorder is static or dynamic. In this paper we study, through numerical simulations, the consequences of the absence of scattering of particular electronic states in the static disorder limit for a one-dimensional system described by Eq. (1.2). We find that, depending on the location of the unscattered state in the parent ordered band, diffusive or super-diffusive transport is obtained. Specifically, if the unscattered state is at the bottom or the top of the band, where it has zero velocity, transport will be diffusive. Super-diffusive transport obtains otherwise.

II. RESULTS

For a one-dimensional system described by Eq. (1.1), the phases of the elements in the basis set of functions can always be chosen so that the off-diagonal matrix elements will be real. By choosing new operators, which are the old operators modulated by a phase,

$$a_m \exp \left[im\theta + i \sum_{n=0}^m \alpha_{n-1, n} \right],$$

where

$$\tan(\alpha_{m-1, m}) = \frac{V \sin(\theta - \phi)}{V \cos(\theta - \phi) + \gamma \Delta_{m-1, m}},$$

the eigenvalue equation for the electronic system in the rigid lattice or Born-Oppenheimer approximation may be written as

$$EC_m = [\varepsilon_0 + G(\Delta_{m+1, m} + \Delta_{m, m-1})]C_m + [V^2 + \gamma^2 \Delta_{m+1, m}^2 - 2\gamma V \Delta_{m+1, m} \cos(\theta - \phi)]^{1/2} C_{m+1} + [V^2 + \gamma^2 \Delta_{m-1, m}^2 - 2\gamma V \Delta_{m-1, m} \cos(\theta - \phi)]^{1/2} C_{m-1}, \quad (2.1)$$

where C_m is the amplitude for the electron to be on site m and E is the energy eigenvalue. We see clearly in (2.1) that any deviations of the lattice ions from equilibrium naturally introduces disorder into the electronic system such that the fluctuations of the diagonal matrix elements and the off-diagonal matrix elements are correlated in a nonlinear fashion. However, a linear relationship between the diagonal and off-diagonal disorder is obtained when $\phi - \theta = 0$ or π . The physical significance of these relationships will be discussed in the following sections.

To analyze the dynamics of an electron obeying (2.1), we calculate the mean-square displacement

$$\overline{m^2} = \sum_m m^2 |C_m(t)|^2 \quad (2.2)$$

by numerically integrating the equations of motion for the site amplitudes for the initial condition $C_0(0) = 1$ for different realizations and amounts of the disorder, using the fourth-order Runge-Kutta method. In order to max-

imize the effect of the disorder, we considered $\gamma\Delta$ to be a spatially independent random variable from a uniform distribution of full width W/V , such that $0 \leq W/V < 2$. The limits on the distribution were set to avoid severing the lattice connections altogether. Calculations were performed on a self-expanding chain to eliminate any edge effects; whenever the probability to be at the ends of the chain exceeded 10^{-30} , ten new sites were added to each end. The results from several random samples are shown in Figs. 1–3. Figure 1 clearly illustrates the tremendous difference between the correlated disorder when $G = \gamma$, and purely diagonal and off-diagonal disorder. In the latter two cases, Fig. 1 illustrates that $\overline{m^2}$ is strongly localized, whereas $\overline{m^2}$ is an increasing function of time for the correlated disorder case. In Fig. 1, $\phi - \theta$ was taken to be zero. In Fig. 2 we compare $\overline{m^2}/Vt$ for values of the disorder ranging from $W/V = 0.5$ to $W/V = 1.9$ for $\phi - \theta = 0$ and $G = \gamma$. The slope of the curves approaches zero at long times, indicating that the transport is diffusive. The more extensive simulation to $Vt = 3000$, in

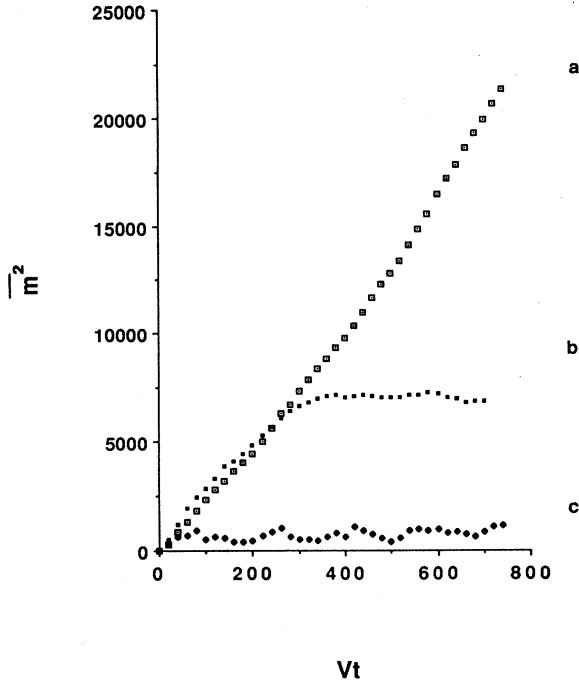


FIG. 1. The mean-square displacement as a function of time (Vt) for site-diagonal, site-off-diagonal, and correlated disorder. The full width of the distribution of the disorder is $W/V=1.0$. The curves are: (a) correlated disorder, (b) site-diagonal disorder, and (c) site-off diagonal disorder. The mean-square displacement is bounded for (b) and (c), indicating localization, and grows with time for (a), indicating diffusion.

the most disordered case ($W=1.9V$), shows clearly that the transport is at least diffusive at long times. Depicted in Fig. 3 is a numerical calculation of $\overline{m^2}/(Vt)^{3/2}$ for an initially localized particle for $G=\gamma$, $W/V=2$, and five

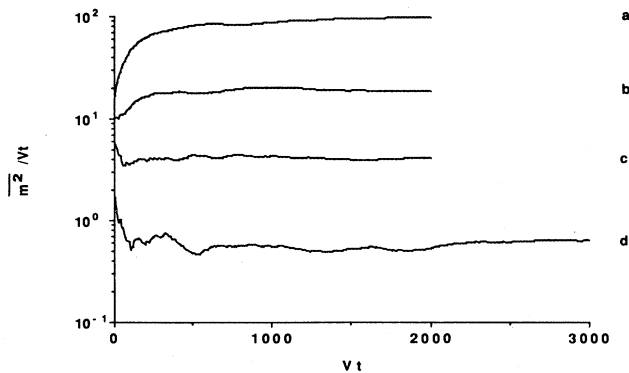


FIG. 2. The mean-square displacement divided by time (Vt), as a function of time, for the case of correlated disorder. The different curves show the response to different amounts of disorder; W/V is (a) 0.5, (b) 1.0, (c) 1.5, and (d) 1.9. The approach to a straight line with zero slope at long times indicates that the process is diffusive.

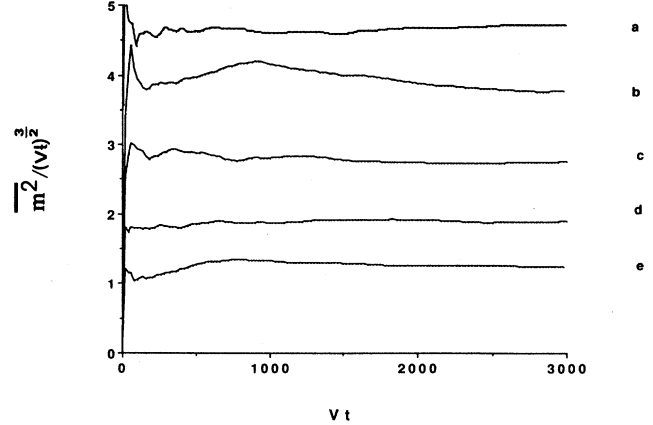


FIG. 3. The mean-square displacement divided by $(Vt)^{3/2}$, as a function of Vt , for the case of perfectly correlated disorder with complex off-diagonal matrix elements. The different curves show the response for different phase angles; $(\phi-\theta)$ is (a) 90° , (b) 60° , (c) 50° , (d) 40° , and (e) 30° . The approach to a straight line with zero slope at long times indicates that the process is superdiffusive. $W/V=2$.

values of the phase difference: $\phi-\theta=30^\circ, 40^\circ, 50^\circ, 60^\circ$, and 90° . The lack of any deviation of $\overline{m^2}/(Vt)^{3/2}$ at long times from a straight line indicates that the mean-square displacement in all of these five cases is indeed growing at $t^{3/2}$. This is the principal result of this paper, namely, that correlations between site and off-diagonal disorder, can give rise to superdiffusion transport even in one-dimension, regardless of the amount of disorder.

III. EXPLANATION OF RESULTS

To explain the numerical results presented in Sec. II, we define A_m to be the amplitude that the electron is in a state created by the operator $a_m^+ \exp(im\theta)$, and let the site energy $\varepsilon_0 = -2V \cos(\phi-\theta)$. The resulting eigenvalue equation is

$$E A_m = (-F_{m+1,m} A_m + F_{m+1,m}^* A_{m+1}) - (-F_{m,m-1} A_{m-1} + F_{m,m-1}^* A_m), \quad (3.1)$$

where

$$F_{m+1,m} = V e^{i(\phi-\theta)} - \gamma \Delta_{m,m+1}.$$

We note that for this choice of phase, the amplitude A_m is conserved; that is, $(d/dt) \sum_m A_m = 0$. The existence of the conservation law for this model suggests that our results may be explained by analogy with corresponding disordered classical models.

Let us begin by considering the case of $\theta=\phi$. The eigenvalue equation that results in negative-semidefinite and equivalent to that of the bond-symmetric disordered master equation.⁸⁻¹¹ Because the eigenvalues are restricted by symmetry to be negative, localized states can

only form below the band. We will see that the states which would normally form localized states above the band edge in the absence of the correlation now remain in the band as current-carrying states in the neighborhood of $E=0$. At this point, we introduce the amplitude flux

$$J_m = F_{m+1,m} (A_m - A_{m+1}),$$

and write (3.1) in the form,

$$E \frac{J_m}{F_{m+1,m}} = -2J_m + J_{m+1} + J_{m-1} \quad (3.2a)$$

or equivalently,

$$E J_m = E \lambda_m J_m + \left\langle \frac{1}{F} \right\rangle^{-1} (-2J_m + J_{m+1} + J_{m-1}), \quad (3.2b)$$

where

$$\lambda_m = \left\langle \frac{1}{F} \right\rangle^{-1} \left[\left\langle \frac{1}{F} \right\rangle - \frac{1}{F_{m+1,m}} \right]. \quad (3.2c)$$

The angular brackets denote a configurational average. We note that, apart from a shift in the energy by an amount $-2V$ Eq. (3.2b) is isomorphic to an equation for the amplitudes with site-diagonal disorder,

$$E C_m = \varepsilon_m C_m + V(C_{m+1} + C_{m-1}), \quad (3.3)$$

if J_m and $\langle 1/F \rangle^{-1}$ in (3.2b) are associated with C_m and V in (3.3), respectively. There is, however, one crucial difference. In (3.2b) the diagonal matrix element, $E \lambda_m$, which now contains the full effect of the correlated disorder, is scaled by the energy. Consequently, for the case of correlated disorder, the states near $E=0$ will show little deviation from Bloch states. The flux-transformed eigenvalue equation for our correlated disorder model is mathematically equivalent to the eigenvalue equation for an isotopically disordered linear chain of harmonic oscillators.¹²⁻¹⁶ As in Eq. (3.3) the energy band of this model is bounded from one side. In the bond disordered master equation the presence of a one-sided energy band results in a branch point of the Green function at $|E|=0$, as evidenced by the nonvanishing of the diffusion constant.⁸⁻¹¹ In the isotopically disordered harmonic chain system, the branch point at $|E|=0$ results from a set of eigenstates in a neighborhood of $|E|=0$, whose localization lengths exceed the system size.¹²⁻¹⁶ In one dimension the early results of Dean and Bacon,¹⁵ Payton and Visscher,¹⁴ and Matsuda and Ishii¹² established that the fraction of such states is of zero measure, and scales as $1/\sqrt{N}$. Matsuda and Ishii¹² have shown for the harmonic-oscillator system that although the width of the unscattered states near $|E|=0$ in one dimension vanishes as the system size grows, such states are nevertheless sufficient in number to give rise to a divergence of the thermal conductivity for particular boundary conditions. Similarly, it is straightforward to show that the number of states with diverging localization lengths is sufficient to give rise to diffusive behavior observed in Sec. II. In one-dimension, states with localization lengths longer than the system size behave as unscattered Bloch states. Their wave vectors k must lie between $k=0$, and $k \sim 1/\sqrt{N}$ as shown by Matsuda and Ishii.¹² Furthermore, they have a mean free path λ on the order of the size of the lattice, $\lambda \sim N$, and

have a velocity $V(k)$ proportional to k at the top of the band. An estimate of the diffusion constant D shows that in the limit that $N \rightarrow \infty$, it remains finite:

$$D = \int V(k) \lambda(k) dk \sim \lim_{N \rightarrow \infty} N \int_0^{1/\sqrt{N}} k dk \sim 1, \quad (3.4)$$

which is in agreement with the long time calculation of the mean-square displacement shown in Fig. 2.

In order to understand the superdiffusive results of Fig. 3 for the case that $\phi \neq \theta$ and $\gamma = G$, it is helpful to compare the density of states, $\rho_d(E)$, of the correlated and disordered system for the special case that $\gamma = G$, with the density of states of the pure crystal, $\rho_0(E)$. We have displayed in Figs. 4(a) and 4(b) an overlay of the numerically calculated densities $\rho_d(E)$ and $\rho_0(E)$ for two cases. In Fig. 4(a) $\phi = \theta$, and in Fig. 4(b) $\phi - \theta = \pi/2$. When

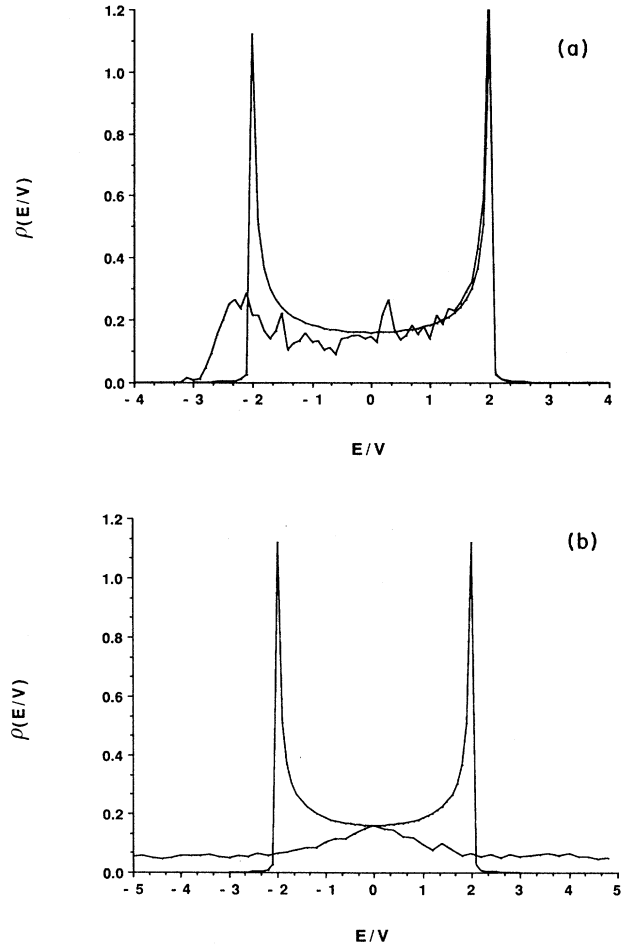


FIG. 4. A comparison of the density of states for the pure linear chain and the density of states for the disordered linear chain, when the disorder is perfectly correlated. The density of states for the disordered system is superimposed upon the density of states for the pure system. In Fig. 4(a), the phase of the off-diagonal matrix elements is zero, $\phi - \theta = 0$, and $W/V = 1$. The density of states is identical to that of the pure system at the upper band edge. In Fig. 4(b), $\phi - \theta = 90^\circ$, and $W/V = 5$. The density of states matches the density of states for the pure system in the middle of the band.

$\phi = \theta$, $\rho_d(E)$ shows no deviation from $\rho_0(E)$ at the band edge, which is in agreement with the previous discussion of the unscattered Bloch states at the band edge. When $\phi - \theta = \pi/2$, however, the point where $\rho_d(E)$ shows no deviation from $\rho_0(E)$ is in the center of the band. In the general case for $\phi \neq \theta$, the energy of the point in the band where $\rho_d(E) = \rho_0(E)$ may be determined by the second term of Eq. (1.2). The unscattered states occur where $k = \theta$, which corresponds to an energy of $2V \cos(\phi - \theta)$. Consequently, the velocity of a particle described by a superposition of such unscattered states is proportional to $2V \sin(\phi - \theta)$. Although the eigenvalue equation in this case lacks the bond symmetry that is obtained when $\phi = \theta$ (and hence is distinct from the disordered harmonic chain), the observation of superdiffusive transport can be explained by assuming that the width of the unscattered states still scales as $1/\sqrt{N}$. In analogy with Eq. (3.4), we compute the diffusion constant by integrating over the number of unscattered Bloch states:

$$D = \int V(k) \lambda(k) dk \sim \lim_{N \rightarrow \infty} N \times \int_{\theta - \phi - 1/\sqrt{N}}^{\theta - \phi + 1/\sqrt{N}} 2V \sin(\theta - \phi) dk \sim \sqrt{N}. \quad (3.5)$$

The unscattered Bloch states traverse a distance on the order of N in a time

$$t \sim \frac{N}{2V \sin(\theta - \phi)},$$

so t and N can be interchanged in Eq. (3.5). Because the diffusion constant is defined as $D = \lim_{t \rightarrow \infty} (d/dt) \bar{m}^2$, we see clearly from (3.5) that wherever $\theta = \phi$ is nonzero, the mean-square displacement will grow as $t^{3/2}$ at long times, as observed in Fig. 3. $\phi = \theta$ is a special limiting case in which bond symmetry obtains and the resultant diffusive transport is described by Eq. (3.4).

IV. PHYSICAL IMPLICATIONS

We first point out that for the length of the simulations we have performed, the particle explores distances on the order of 500 to 1000 lattice constants. In addition, for a typical solid $Vt \sim 3000$ corresponds to times comparable to the inelastic scattering time. Hence, in a real material, the motion predicted here will be distinct from hopping transport where the mean free path is of the order of a lattice constant.

In the Anderson model of site-diagonal disorder, in higher dimensions, when the amount of disorder W exceeds a critical value W_c , all of the states in the system are localized except possibly for a set of delocalized states of measure zero.^{1,2} It is easy to see for the case of correlated disorder with $\phi = \theta$, however, that the critical value W_c tends to infinity. From the d -dimensional eigenvalue equation for the fluxes

$$EJ_m^v = E\alpha_m^v J_m^v + \left\langle \frac{1}{V^v} \right\rangle^{-1} \sum_{\mu} (J_{m-\mu}^{\mu} + J_{m+\mu}^{\mu} - 2J_m^{\mu}), \quad (4.1)$$

for the amplitude flux J_m^v , it is clear that in any dimension because the disorder α_m^v along the v th direction

scales with the energy, the states near $E = 0$ will be perturbed by an effectively reduced amount of disorder. Thus, given a value of $W > W_c$, which would cause complete localization of the states of (3.3), a value of E can always be found in the correlated case such that, in (8) $|EW| < W_c$, thereby suppressing the Anderson transition for a finite value of W . We believe this result still holds when $\phi \neq \theta$, although we have not been able to construct an equation of the form of (4.1) for this case. We reiterate that the source of delocalization or transport in this model is a set of states of zero measure whose localization lengths are longer than the system size. It is worth reemphasizing that the standard analyses¹⁻⁵ of Anderson localization do not preclude the presence of a set of states of zero measure at a particular energy whose localization lengths diverge. For example, a calculation of the imaginary part of the self-energy (as in Ref. 2) for correlated disorder reveals that the self-energy tends to zero regardless of the energy. That is, a set of states of zero measure is insufficient to give rise to a branch point along the $\text{Re}E$ axis. Under usual circumstances, this state of affairs would signify an absence of transport. However, for correlated disorder, the fraction¹² ($1/\sqrt{N}$) of such states with localization lengths longer than the system size is sufficiently great that they give rise to transport. The fraction of the particle wave function that is formed from the electronic states whose localization lengths diverge moves through the lattice ballistically and ultimately gives rise to superdiffusion. That such a state of affairs could arise does not appear to have been previously anticipated.

We see then that correlations between the site-diagonal and site off-diagonal matrix elements of the type discussed here lead to superdiffusion in one-dimension and ultimately suppress the Anderson transition (for finite W) in higher dimensions. Hence, our results are in stark contrast to the presently held view that transport can only obtain in a disordered system for $d > 2$.⁵ It is important then to determine under what circumstances the behavior predicted here can be experimentally observed. We first note that as the phase angle $(\theta - \phi)$ is varied, Eq. (2.1) describes a wide range of correlations between the site energies and the transfer-matrix elements. For example, when $0 < |\theta - \phi| < \pi/2$, Eq. (2.1) indicates that the correlations between ϵ_n and $V_{n,n\pm 1}$ are such that when two neighboring ions move closer together, the transfer-matrix element increases and the site energy decreases. In the regime $\pi/2 < |\theta - \phi| < \pi$, the transfer-matrix element decreases the more tightly bound an electron is on a given site. In either case, perfect correlation ($\gamma = G$) between ϵ_n and $V_{n,n\pm 1}$ ensures that an unscattered state will persist in the band at a value of the dimensionless wave vector $k = \theta - \phi$ and if $k \neq 0$, then $\bar{m}^2 \sim t^{3/2}$. This result is true whether the disorder is static or dynamic. A quasideimensional material possessing such perfect correlations will exhibit the enhancement in conductivity ($\bar{m}^2 \sim t^{3/2}$) if the Fermi level coincides with the position of the unscattered state in the band. Successive doping of a material until Fermi level coincides with the unscattered state should result in a marked increase in the conductivity if perfect correlations between ϵ_n and $V_{n,n\pm 1}$

are present. GaAs heterostructures, which can be grown layer by layer using molecular beam epitaxy to possess a specified arrangement of quantum wells of varying thickness and depth¹⁷ may be ideal systems for seeing the effects of correlations between ε_n and $V_{n,n\pm 1}$.

In systems in which control over ε_n and $V_{n,n\pm 1}$ is less than ideal it is important to understand what role the correlations, which are naturally present, play in determining the transport properties. Equation (2.1) suggests a straightforward extension of our results from the perfectly correlated ($\gamma = G$) case to the regime $\gamma \neq G$. When the disorder is small relative to the parent bandwidth, $G\Delta_{m,m+1} < 4V$, the square root in (2.1) can be expanded in powers of $G\Delta_{m+1,m}/V$. To linear order in $G\Delta_{m+1,m}/V$ in the perfectly correlated case, Eq. (2.1) becomes

$$\begin{aligned} EC_m = & [\varepsilon_0 + G(\Delta_{m+1,m} + \Delta_{m,m-1})]C_m \\ & + [V - G \cos(\theta - \phi)\Delta_{m+1,m}]C_{m+1} \\ & + [V - G \cos(\theta - \phi)\Delta_{m,m-1}]C_{m-1}. \end{aligned} \quad (4.2)$$

Equation (4.2) is the approximate eigenvalue expression for the perfectly correlated case for small relative displacements of the ions. In the linear regime then, the effective off-diagonal coupling constant γ is equal to $G \cos(\theta - \phi)$, or more importantly, $|\gamma| \leq |G|$. Consequently, when the disorder is small, the stringent condition that γ must equal G for the presence of an unscattered state is no longer necessary. When $|\gamma| \leq |G|$, an unscattered state will exist in the parent-ordered band at an energy $2V \cos(\theta - \phi)$, that is, $2V\gamma/G$, and furthermore, for $|\gamma| < |G|$ the mean-square displacement will grow as $t^{3/2}$. Of course, this result is only true at times short enough so that the effect of the terms to second order in $G\Delta_{m+1,m}/V$ may be neglected. An example of this behavior is shown in Fig. 5, where we have calculated $\overline{m^2}/Vt$ from Eq. (4.2) for three cases: (a) the perfectly correlated case of $\gamma = G = 0.5$, (b) an imperfectly correlated case $\gamma = 0.4$ and $G = 0.5$, and (c) an imperfectly correlated case $\gamma = 0.5$ and $G = 0.4$; $W/V = 1$. For the time scale considered, the imperfectly correlated case (b) behaves as though it were perfectly correlated, with the less-strongly-localized states contributing to a nonzero velocity. We see that, although the mean-square displacement increases as t for the perfectly correlated case, $|\gamma| = |G|$, on the same time scale it increases even faster, as $t^{3/2}$, for $|\gamma| < |G|$. This result is certainly surprising, and illustrates the resilience of the perfectly unscattered states to weak off-diagonal perturbations. On the other hand, the imperfectly correlated case (c) for $|\gamma| > |G|$ is subdiffusive for this time scale, showing a stronger localization than case (a). Thus, if the dominant source of scattering is due to electron-photon interactions, a sharp rise in the dc conductivity should occur when the Fermi energy matches $2V\gamma/G$, provided that the off-diagonal electron-phonon coupling is weaker than the diagonal electron-phonon coupling, and that temperatures are sufficiently low so that the electron-phonon interaction is small compared with the bandwidth. Once the energy of

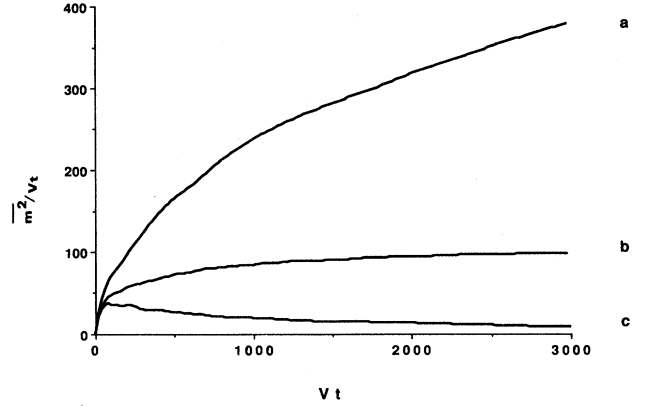


FIG. 5. The mean-square displacement divided by Vt , as a function of Vt , for correlated disorder with off-diagonal matrix elements which have been linearized in the relative displacements Δ of the ions. The perfectly correlated case (b) for $W = \gamma\Delta = G\Delta = 0.5V$ gives rise to diffusion. However, in the imperfectly correlated case (a) for $\gamma\Delta = 0.4V$, $G\Delta = 0.5V$, the transport is much faster for this time scale, with the mean-square displacement growing as $t^{3/2}$. In the imperfectly correlated case (c) for $\gamma\Delta = 0.5V$, $G\Delta = 0.4V$, localization is stronger, and transport is subdiffusive.

the unscattered states and the parent bandwidth $4V$ have been determined, the relative strengths of the off-diagonal and diagonal electron-phonon coupling in a particular sample can be obtained. We note in passing that, when the off-diagonal coupling constant is zero, the least-localized states are in the middle of the band at $E = 0$. This is in agreement with the results for systems with purely site-diagonal disorder.⁴

In the preceding discussion we have treated the disorder as a continuous variable. That is, we have allowed the relative displacements of the ions to range freely within the bounds of a distribution. In some cases, however, especially at low temperatures, strain defects may be found in very limited varieties. Consider, for example, a case in which the nearest-neighbor pair potential has two minima, as in glasses.¹⁸ There are defects in such samples in the sense that one or the other minima may be occupied in an irregular fashion throughout the material. To model systems of this type, let us treat the normal ion-separation as the position of one of the minima, and the defect ion separation to be at the position of the other minima, a distance Δ away. The off-diagonal matrix element between sites m and $m + 1$ is in general some function $g(X_m - X_{m+1})$, and the diagonal matrix element for site m is the sum of the interactions with the nearest neighbors to the left and to the right of m ,

$$f(X_m - X_{m+1}) + f(X_{m-1} - X_m).$$

The functions f and g may be nonlinear and are functions only of the relative displacement between nearest neighbors $X_m - X_{m+1}$. Note that $X_m - X_{m+1}$ need not necessarily correspond to a linear displacement. In systems with more than one atom per unit cell, $X_m - X_{m+1}$ could

correspond to a rotation of one cell relative to the other. Nonetheless, f and g will be evaluated for only two values of the argument: $X_m - X_{m+1} = 0$ or Δ . The eigenvalue equation for the system is

$$EC_m = [\varepsilon_0 + f(X_m - X_{m+1}) + f(X_{m-1} - X_m)]C_m + g(X_m - X_{m+1})C_{m+1} + g(X_{m-1} - X_m)C_{m-1}. \quad (4.3)$$

Depending on the relative magnitudes of $f(X_m - X_{m+1})$ and $g(X_{m-1} - X_m)$, the mean-square displacement of the correlated system described by (4.3) will *quite generally* be either bounded, or grow superdiffusively, as $t^{3/2}$. To see this, we map (4.3) into the form of (2.1) by solving for the constants V , ε_0 , and Φ such that the following two equations are satisfied:

$$\{V^2 + [f(0) + \varepsilon_0/2]^2 - 2V[f(0) + \varepsilon_0/2]\cos(\Phi)\}^{1/2} = g(0), \quad (4.4a)$$

$$\{V^2 + [f(\Delta) + \varepsilon_0/2]^2 - 2V[f(\Delta) + \varepsilon_0/2]\cos(\Phi)\}^{1/2} = g(\Delta). \quad (4.4b)$$

If a solution to the system of Eqs. (4.4a) and (4.4b) exists, then the motion predicted by (4.3) will be indistinguishable from the motion predicted by (2.1) in the perfectly correlated case. Namely, the localization lengths will

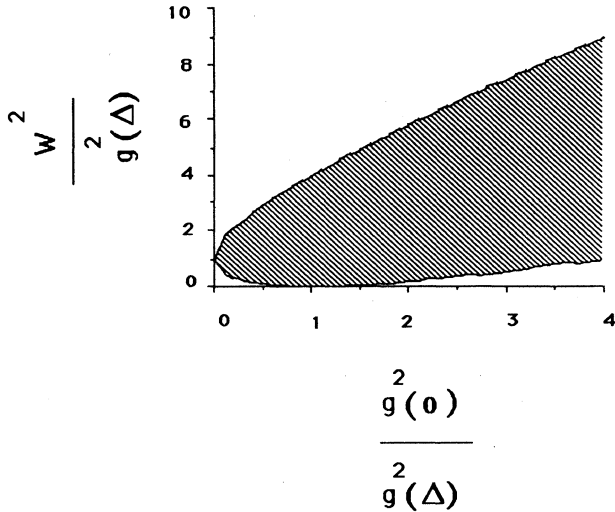


FIG. 6. The phase diagram for the two-state correlated model. If the point located by particular values of the parameters W , $g(0)$, and $g(\Delta)$ lies within the shaded region, motion is superdiffusive. Points lying on the boundary of the shaded region, correspond to diffusive motion. The mean-square displacement is bounded for all points lying outside the shaded region.

diverge for states with energy tending to $2V \cos(\Phi)$, and the mean-square displacement will increase as $t^{3/2}$ (unless Φ is zero or π , in which case diffusion occurs). If a solution to the system (4.4a) and (4.4b) does not exist however, there will be some scattering of every Bloch state. In this case, every state will be exponentially localized with a finite localization length, and the mean-square displacement will remain bounded at long times. Thus, there is a transition from subdiffusive transport to superdiffusive transport in the one-dimensional system. In order to describe the transition point, we consider the case in which the probability of finding a defect separation (Δ) is P , and the probability of finding a normal (zero) separation between the ions is $1-P$. Without loss of generality, we choose the arbitrary constant ε_0 ,

$$\varepsilon_0 = 2[(P-1)f(0) - Pf(\Delta)] \quad (4.5)$$

such that the average of $(f + \varepsilon_0)/2$ is zero. After a little algebra, we find that the constants V and Φ are given by

$$V = [Pg(\Delta)^2 + (1-P)g(0)^2 - W^2(1-P)P]^{1/2}, \quad (4.6)$$

$$\Phi = \cos^{-1} \left[\frac{1}{2V} \left[\frac{g(0)^2 - g(\Delta)^2 - (2P-1)W^2}{W} \right] \right], \quad (4.7)$$

provided that the condition

$$W^4 + [g(0)^2 - g(\Delta)^2]^2 \leq 2W^2[g(0)^2 + g(\Delta)^2] \quad (4.8)$$

is satisfied. The full width of the diagonal disorder $W = f(\Delta) - f(0)$. Condition (4.8) defines a region in which the parameters W , $g(\Delta)$, and $g(0)$ must lie in order for the transport to be superdiffusive. This region is shown explicitly in Fig. 6. For parameters outside the region, the mean-square displacement is bounded. If the parameter lie on the boundary, the mean-square displacement grows as t . For parameters within the region, however, the mean-square displacement grows as $t^{3/2}$. We remark that for the special case that $g(\Delta) = g(0) = v$, the description of the boundary between superdiffusion and the absence of diffusion is considerably simpler. In this case, the boundary is located at $W = 2v$. For $W < 2v$ transport is superdiffusive. When $W = 2v$, transport is diffusive, and if $W > 2v$, there is no transport at all. We note that Eq. (4.8) does not depend on P . Hence, the transition point depends only on the magnitude of the defects, and not on their concentration. The behavior predicted here should be experimentally observable in quasioone-dimensional materials such as conducting polymers in which the dominant disorder is structural and is described for the most part by a bivalued distribution.

V. FINAL REMARKS

In closing, we have presented an electronic system in which correlations between diagonal and off-diagonal matrix elements lead to an absence of localization of an initially localized particle. We have shown that superdiffusive transport can obtain in this one-dimensional system, regardless of the magnitude of the disorder when the unscattered state in the band has a

finite velocity. Such transport in the perfectly correlated case was shown to be resilient to weak off-diagonal perturbations. As a result then, the experimental circumstances under which the behavior predicted here can be observed are quite general. In addition to GaAs heterostructures which can be designed to test the predictions of the perfectly correlated model, quasi-one-dimensional systems such as phthalocyanine macrocyclic compounds,¹⁹ in which the position of the Fermi level is easily tuned, are likely candidates for testing the general predictions of correlated phonon disorder. In addition to enhancing the conductivity in disordered systems, correlated disorder can also serve as a probe of the relative magnitudes of the diagonal and off-diagonal electron-phonon coupling constants.

Because many more paths are available, it is likely that transport in a higher-dimensional system with correlated disorder will be faster. Our preliminary calculations for

the case in which the unscattered state lies at the top of the band indicate that based on the exponential divergence¹¹ of the localization length near $E=0$ and the zeroth-order estimate of the mean free path [$\lambda(k) \sim k^{-(d+1)}$] that, in two dimensions, the diffusion coefficient diverges as $\ln(N)$. Further work is needed to fully extend the analysis presented here to higher-dimensional systems.

ACKNOWLEDGMENTS

The authors wish to thank U. Mohanty and R. Field for donating invaluable computer time, and the National Science Foundation (NSF) for funding this work. They are grateful to Paul Parris, Morrel Cohen, Patrick Lee, George Tsironis, David E. Logan, and Stuart Trugman for helpful comments and discussions.

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