Absence of Localization in a Random-Dimer Model

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We consider here a 1D tight-binding model with two uncorrelated random site energies ϵ_a and ϵ_b and a constant nearest-neighbor matrix element V. We show that if one (or both) of the site energies is assigned at random to pairs of lattice sites (that is, two sites in succession), an initially localized particle can become delocalized. Its mean-square displacement at long times is shown to grow in time as $t^{3/2}$ provided that $-2V<\epsilon_a-\epsilon_b<2V$. Diffusion occurs if $\epsilon_a-\epsilon_b=\pm 2V$ and localization otherwise. The dual of the random-dimer model is also shown to exhibit an absence of localization and is shown to be relevant to transmission resonances in Fibonacci lattices.

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The Anderson model for site-diagonal disorder has proven to be of fundamental importance in our understanding of the role disorder plays in insulator-metal transitions in a wide range of materials, most notably Si:P.[1,2] A well-known result of the Anderson model for site-energy disorder is the vanishing of the diffusion constant of an initially localized particle for any amount of disorder in one and two dimensions. In this paper, we consider probably the simplest tight-binding model that exhibits Anderson localization. We focus on a one-dimensional tight-binding model of a random binary alloy in which the site energies ϵ_a and ϵ_b are assigned at random to the lattice sites with probability q and $1-q$, respectively. A constant nearest-neighbor matrix element V mediates transport between the lattice sites. In one dimension, it is well accepted that for all nonzero q, all the eigenstates will be exponentially localized and no long-range transport will be observed at long times.[3]

Consider, for the moment, a particular realization of the site energies in a certain segment of the infinite lattice: $\ldots\epsilon_a\epsilon_a\epsilon_b\epsilon_a\epsilon_a\epsilon_a\epsilon_b\epsilon_b\epsilon_a\epsilon_b\epsilon_b\epsilon_b\epsilon_b\epsilon_a\ldots$. Given the rigorous nature of the theorems establishing quasiparticle localization in one-dimension, it seems safe to assume that the one-dimensional results are not only independent of q, but also of the number of ϵ_a's or ϵ_b's that appear in clusters in the lattice. That is, the localization of one-dimensional quasiparticles still persists if all clusters containing an odd number of ϵ_b's are replaced by clusters containing an odd number of ϵ_a's, for example. After all, under such a transformation, the system is still random and the localization theorems guarantee an absence of transport for any degree of randomness in one dimension. We show here that this is *not* the case. In particular, we show that when one of the site energies is assigned at random to pairs of lattice sites (that is, two sites in succession), $\sqrt{N}$ of the electronic states are extended over the entire sample. In addition, we show that the tight-binding model that describes this system is equivalent to a simplified version of the correlated disorder model recently proposed by Dunlap, Kundu, and Phillips (DKP).[4] We refer to a lattice in which *at least* one of the site energies is assigned at random to pairs of lattice sites as the random-dimer model. We show by numerical simulation that the mean-square displacement of an initially localized particle in the random-dimer model will grow as $t^{3/2}$ provided that $-2V<\epsilon_a-\epsilon_b<2V$. Diffusion is shown to occur when $\epsilon_a-\epsilon_b=\pm 2V$. In all other cases, the particle remains localized at long times. Our results are shown to be valid even when both ϵ_a and ϵ_b are individually assigned at random to pairs of lattice sites. This case is certainly more surprising than the former because it seems reasonable to assume that such a system is equivalent to the completely random binary alloy with two sites per unit cell. Here again, we show that this is not the case. We close by showing how an absence of localization can occur in a random two impurity model even when the pairing constraint is relaxed. The connection between such a model and transport in Fibonacci lattices[5] is discussed. This work certainly suggests that a number of physically relevant models might exist that exhibit an absence of localization.

To determine the dynamics of an electron in the random-dimer model (RDM), we numerically integrated the equations of motion,

$$i\dot{c}_n=\epsilon_n C_n+V(C_{n+1}+C_{n-1}), \tag{1}$$

for the site amplitudes $C_n(t)$ and calculated the mean-square displacement,

$$\overline{m^2}=\sum_m m^2|C_m|^2. \tag{2}$$

Our calculations were performed on a self-expanding chain with the localized initial condition $C_0(t=0)=1$. The self-expanding chain was used to minimize end effects; whenever the probability of finding the particle 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 Fig. 1. The site energies were chosen from the bivalued distribution $\epsilon_n=\epsilon_a$ and $\epsilon_n=\epsilon_b$ with $q=\frac{1}{2}$. This choice of q corresponds to the most disordered case. Figure 1 compares the mean-square displacement in the random-dimer model for three different values of $\epsilon_a-\epsilon_b$: (a) $\epsilon_a-\epsilon_b=V$, (b) $\epsilon_a-\epsilon_b=2V$, and (c) $\epsilon_a-\epsilon_b=3V$. The dotted curves are the

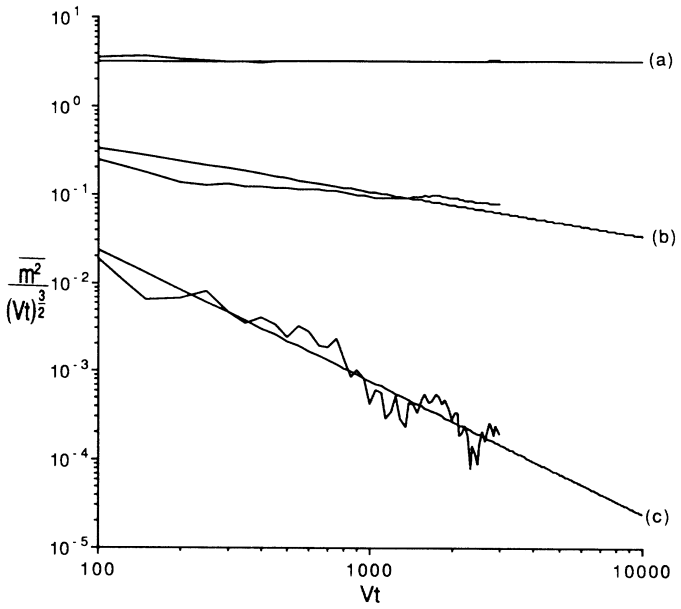

FIG. 1. The mean-square displacement divided by $(Vt)^{3/2}$ for varying amounts of disorder in the random-dimer model: (a) $\epsilon_a-\epsilon_b=V$, (b) $\epsilon_a-\epsilon_b=2V$, and (c) $\epsilon_a-\epsilon_b=3V$. The mean-square displacement grows as $t^{3/2}$ in case (a), linearly as t in (b), and is bounded for (c).

data from single numerical simulations, whereas least-squares fits of the data with an expression of the form $\overline{m^2}=A(Vt)^b$ are represented by solid lines. The constant A was allowed to vary, while the exponent b was set to $\frac{3}{2}$, 1, and 0 for the cases (a), (b), and (c), respectively. The subsequent straight-line fit through the data in each of these cases indicates that the transport properties are as advertised, namely, superdiffusive for $-2V<\epsilon_a-\epsilon_b<2V$, diffusive for $\epsilon_a-\epsilon_b=\pm 2V$, and localized otherwise. We emphasize that we have considered the most disordered case, $q=\frac{1}{2}$. Hence, the results reported here could only be enhanced as the disorder is decreased.

Probably the simplest way to understand our results is to consider an otherwise ordered lattice with a single dimer defect. Let us place the dimer on sites 0 and 1. We assign the energy ϵ_a to all the sites except sites 0 and 1. Let the energy of sites 0 and 1 be ϵ_b. A constant nearest-neighbor matrix element V mediates transport between the sites. We first show that $\sqrt{N}$ of the electronic states are unscattered by the dimer impurity. Then, we construct explicitly the unscattered states in a lattice containing randomly placed dimers. To proceed we calculate the reflection and transmission coefficients through the dimer impurity. Let us write the site amplitudes as $C_n=e^{ikn}+Re^{-ikn}$ for $n\leq -1$ and $C_n=Te^{ikn}$ for $n\geq 1$, where R and T are the reflection and transmission amplitudes, respectively. From the eigenvalue equation for sites -1 and 1, it follows that $C_0=1+R=T(\epsilon_- e^{-ik}+V)/V$ with $\epsilon_-=\epsilon_a-\epsilon_b$. Substitution of this result into the eigenvalue equation for site 0 results in the following closed expression:

$$|R|^2=\frac{\epsilon_-^2(\epsilon_-+2V\cos k)^2}{\epsilon_-^2(\epsilon_-+2V\cos k)^2+4V^4\sin^2 k} \tag{3}$$

for the reflection probability. The reflection coefficient vanishes then when $\epsilon_a-\epsilon_b=-2V\cos k$ or equivalently when $-2V\leq\epsilon_a-\epsilon_b\leq 2V$. We point out that when this condition holds, or equivalently when $E(k)=\epsilon_b$, the product of a pair of b transfer matrices yields the unit matrix. Under such conditions, Furstenberg's theorem implies that the electronic state at that energy will be extended.[6] The location in the parent-ordered band of the perfectly transmitted electronic state corresponds to the wave vector $k_0=\cos^{-1}[(\epsilon_b-\epsilon_a)/2V]$. Of course, no transport would occur if only a single electronic state remained unscattered. To determine the total number of states that behave in this fashion, we expand R around k_0. To lowest order we find that in the vicinity of k_0, $|R|^2\sim(\Delta k)^2$ where $\Delta k=k-k_0$. Consider now a crystal containing a certain fraction of randomly placed dimer impurities. Electronic states in the vicinity of k_0 will be reflected with a probability proportional to $(\Delta k)^2$. The time between scattering events τ is inversely proportional to the reflection probability.[7] As a result, in the random system, the mean free path $\lambda=\langle v\rangle\tau\sim 1/(\Delta k)^2$ in the vicinity of k_0, where v is the velocity.[7] Let $\Delta k=\Delta N/2\pi N$. Upon equating the mean free path to the length of the system (N), we find that the total number (ΔN) of states whose mean free path is equal to the system size scales as $\Delta N=\sqrt{N}$. Because the mean free path is approximately equal to the localization length in one dimension, we find that the total number of states whose localization lengths diverge is $\sqrt{N}$. Consequently, in the random-dimer model $\sqrt{N}$ of the electronic states remain extended over the total length of the sample. Such states move through the crystal ballistically with a constant group velocity [$v(k)$] except when they are located at the bottom or the top of the band where the velocity vanishes. Because all the other electronic states are localized, the diffusion constant is determined simply by integrating $v(k)\lambda(k)$ over the width of k states that participate in the transport. The upper limit of the integration is then proportional to the total fraction of unscattered states or $1/\sqrt{N}$ and $\lambda(k)\sim N$. In the case when the velocity is a nonzero constant, we obtain that $D\sim\sqrt{N}$. Because the states which contribute to transport traverse the length of the system with a constant velocity, t and N can be interchanged or $D\sim t^{1/2}$. Consequently, the mean-square displacement grows as $t^{3/2}$. At the bottom or the top of the band where the group velocity vanishes, $v(k)\sim k$ and $D\sim 1$.

We now construct explicitly the unscattered states. In absence of any dimer impurities, the eigenstates are simply Bloch states of the form e^{ikn}. When the dimer impurities are present because the eigenstates in the vicinity of k_0 have unit transmission, it must be the case that

these states are still of the Bloch form. These states can be constructed as follows: Consider the single-dimer impurity case discussed earlier. The dimer impurity is located on sites 0 and 1. The unscattered state must be of the form e^{ikn} for $n \leq 0$ and $e^{ikn+i\Omega}$ for $n \geq 1$. That is, the only difference between the electron wave function before and after it has interacted with the impurity is that its phase changes by Ω. There is no reflected component. To determine Ω, we consider the eigenvalue equation $E-\epsilon_b = V(e^{ik+i\Omega}+e^{-ik})$ for site 0. This equation has a trivial solution when $\epsilon_a = \epsilon_b$ or equivalently in the limit of an ordered system. In this case $\Omega = 0$. The nontrivial solution occurs when $E-\epsilon_b = 0$. Recall that when $E-\epsilon_b = 0$, the reflection coefficient vanishes and the product of two b-type transfer matrices yields the unit matrix. Because E is the energy of the ordered band, $\epsilon_a + 2V\cos k$, the vanishing of $E-\epsilon_b = 0$ corresponds to the condition $-2V \leq \epsilon_a - \epsilon_b \leq 2V$. In this case, $\Omega = -2k+\pi$. Consequently, the Bloch state that satisfies the Schrödinger equation is e^{ikn} for $n \leq 0$ and $-e^{ik(n-2)}$ for $n \geq 1$ provided that $-2V \leq \epsilon_a - \epsilon_b \leq 2V$. The wave function on the second atom of the dimer is the negative of the a-type atom located on site -1. The unscattered state then is odd with respect to reflection around the first atom of the dimer. If another dimer were located on sites 2 and 3, the corresponding perfectly transmitted wave would be $\ldots e^{-2ik}, e^{-ik}, 1, -e^{-ik}, -1, e^{-ik}, 1, e^{ik}, e^{2ik}, \ldots$ provided, of course, that $-2V \leq \epsilon_a - \epsilon_b \leq 2V$. Such states can always be constructed regardless of the number of dimer impurities that are placed at random in the lattice. Although the phase changes as the electron scatters from a dimer impurity, there is no reflection for $\sqrt{N}$ of the electronic states. It is straightforward to verify that similar states cannot be constructed for single impurities in the absence of off-diagonal disorder. We show in Fig. 2 a graph of the real part of a perfectly transmitted electronic state at a particular value of k as a function of the concentration of dimers. As is evident, the electronic state is extended although "scattering" occurs at each dimer. This is the principal result of this paper.

The only remaining question in the RDM is the exact location of the set of perfectly transmitted electronic states in the energy band of the disordered system. To answer this question we consider the correlated disorder model of DKP. The essence of the DKP model is that any system described by a tight-binding Hamiltonian of the form

$$H = \sum_{\mathbf{n}} \epsilon_{\mathbf{n}} a_{\mathbf{n}}^{\dagger} a_{\mathbf{n}} + \sum_{\mathbf{n},\mu} V_{\mu;\mathbf{n},\mathbf{n}+\mu} (a_{\mathbf{n}}^{\dagger} a_{\mathbf{n}+\mu} + a_{\mathbf{n}+\mu}^{\dagger} a_{\mathbf{n}}) \quad (4)$$

will exhibit superdiffusive transport if the site energies and transfer-matrix elements can be written as

$$\epsilon_{\mathbf{n}} = \sum_{\mu} (G_{\mu;\mathbf{n},\mathbf{n}+\mu} + G_{\mu;\mathbf{n},\mathbf{n}-\mu}) \quad (5)$$

and

$$V_{\mu;\mathbf{n},\mathbf{n}\pm\mu} = (V_{\mu}^2 + G_{\mu;\mathbf{n},\mathbf{n}\pm\mu}^2 - 2G_{\mu;\mathbf{n},\mathbf{n}\pm\mu} V_{\mu} \cos\theta_{\mu})^{1/2}, \quad (6)$$

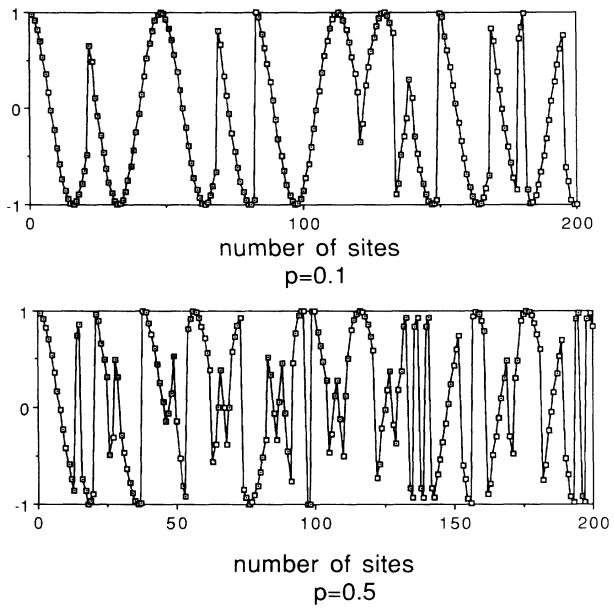

FIG. 2. The real part of the unscattered eigenstate in the random-dimer model. p is the concentration of dimers. The wave function moves through the crystal with a phase that is randomized at each dimer impurity. No backscattering occurs, however, when $-2V \leq \epsilon_a - \epsilon_b \leq 2V$.

respectively. In Eqs. (4)–(6), $a_{\mathbf{n}}^{\dagger}$ creates an electron at a site with direct lattice vector $\mathbf{n}$, μ is a positive unit vector originating at $\mathbf{n}$ pointing to the nearest-neighbor sites along the μth direction of the crystal, V_{μ} is the bare bandwidth along the μth direction, and $G_{\mu;\mathbf{n},\mathbf{n}\pm\mu}$ is a random-bond variable connecting sites $\mathbf{n}$ and $\mathbf{n}\pm\mu$. In the context of structurally induced disorder, $G_{\mu;\mathbf{n},\mathbf{n}\pm\mu}$ was shown to be some function (linear or otherwise) of the relative displacement between ions located at $\mathbf{n}$ and $\mathbf{n}\pm\mu$. It was shown that if Eqs. (5) and (6) apply, an unscattered state will exist with wave vector $\mathbf{k} = \boldsymbol{\theta}$ in the parent-ordered band.[4] The total fraction of states in the vicinity of $\mathbf{k} = \boldsymbol{\theta}$ that remains unscattered scales as $1/\sqrt{N}$.[4] To apply this model to the problem at hand, we note that the site energies in the random-dimer model can be constructed from a constrained bivalued distribution of G's—that is, from a distribution of the form $G_{n,n\pm1} = G_a$ and $G_{n,n\pm1} = G_b$ with probabilities P and $1-P$, respectively. Because the site energies are of the form $\epsilon_n = G_{n,n+1} + G_{n,n-1}$, the constraint that must be imposed is that G_b, for example, cannot occur consecutively in the lattice. The resultant site energies will be $\epsilon_a = 2G_a$ and $\epsilon_b = G_b + G_a$ with the ϵ_b's occurring in pairs. The matrix elements that are generated by G_a and G_b must, of course, be equal in the RDM. Solving the two simultaneous equations that result from Eq. (6) for the $\cos\theta$ term, makes the matrix elements equal yields the general condition for the location of the unscattered state,

$$\cos\theta = \frac{1-3q}{2[(V/W)^2(1+q)^2 - 2q(1-q)]^{1/2}}, \quad (7)$$

where q is the concentration of ϵ_a. The location of the unscattered state is then a function of the concentration as well as the relative disorder V/W with $W=\epsilon_a-\epsilon_b$. Substitution of the restriction $-1\leq\cos\theta\leq 1$ into (7) yields the general result that $-1\leq W/2V\leq 1$ for an unscattered state to exist. We note that when $\epsilon_a-\epsilon_b=\pm 2V$, $\cos\theta=\pm 1$ regardless of the concentration q. In this case, the unscattered states have zero velocity and diffusion occurs. For all other values of W, provided that $-1\leq W/2V\leq 1$, the location of the unscattered states depends on q and will have a nonzero velocity.

We note in closing that it is possible for the absence of localization to persist even when the pairing constraint is relaxed. Consider a lattice containing two types of impurities with energies ϵ_a and ϵ_b with the constraint that the b-type impurities do not occur on neighboring lattice sites. Let V_a be the nearest-neighbor matrix element connecting two sites with energy ϵ_a and V_b the overlap of two sites with energy ϵ_a and ϵ_b. In such a lattice, the V_b-type matrix elements occur in pairs and hence this model is the dual of the random-dimer model. It is straightforward to show that in this model the reflection coefficient through a single b impurity will vanish provided that $V_a|\epsilon_a-\epsilon_b|\leq 2|V_a^2-V_b^2|$. Using arguments analogous to those used in the RDM, we find also that $\sqrt{N}$ of the electronic states are extended when this condition holds. The phases of the unscattered states in this model, however, do not change. The amplitude changes by the ratio V_a/V_b when an impurity is encountered. For example, if b-type impurities are located on sites -1 and 2, the unscattered eigenstate is $\ldots e^{-2ik}$, $(V_a/V_b)e^{-ik}$, 1, e^{ik}, $(V_a/V_b)e^{2ik}$, e^{3ik}, ... The arrangement of the layers in Fibonacci lattices[5] fabricated from two types of materials (such as GaAs and AlAs) is a subclass of the disorder inherent in the single-impurity model described above. In such systems transmission resonances should be observed at particular energies when the criterion described above holds. In a forthcoming paper,[8] we discuss in detail the relationship between such quasiperiodic systems and the single-impurity model.

We have presented some simple models which possess surprising localization-delocalization transitions. Transport in these models occurs because $\sqrt{N}$ of the electronic states are extended over the whole sample. Any physical system that can be described either by the RDM or the single-impurity model (such as Fibonacci lattices) should exhibit transmission resonances and a drastic enhancement in its conductivity when the Fermi level coincides with the position of the unscattered states. Hence, these models could be used to guide the synthesis of new highly conductive materials. As we have discussed earlier,[4] the standard localization theorems[1-3] are completely consistent with the occurrence of a set of delocalized states of zero measure. Such states do not affect the vanishing of the imaginary part of the self-energy along the ReE axis, for example. What is surprising here is that they are of sufficient number $\sqrt{N}$ to give rise to transport. Pendry[9] has shown that in standard disordered models, isolated states at particular energies remain extended over $\sqrt{N}$ of the lattice sites. However, the number of states which behave in this fashion is exponentially small.[9] As a result, such states do not affect the asymptotic value of the mean-square displacement of an initially localized particle, in contrast to the extended states in the RDM. It is straightforward to verify that in higher dimensions, an absence of localization still persists. Although the precise time dependence of the mean-square displacement is not known, we are guaranteed that it is at least $t^{3/2}$.

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Note added.—While this work was in progress a paper appeared by Flores[10] showing similar results for the dilute binary alloy.

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