Unusual properties of midband states in systems with off-diagonal disorder

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It is known that off-diagonal disorder results in anomalous localization at the band center, whereas diagonal disorder does not. We show that the important distinction is not between diagonal and off-diagonal disorder, but between bipartite and nonbipartite lattices. We prove that bipartite lattices in any dimension (and some generalizations that are not bipartite) have zero energy (i.e., band-center) eigenfunctions that vanish on one sublattice. We show that $\ln|\psi_j|$ has random-walk behavior for one-dimensional systems with first-, or first- and third-neighbor random hopping, leading to $\exp(-\lambda\sqrt{r})$ localization of the zero-energy eigenfunction. Addition of diagonal disorder leads to a *biased* random walk. First- and second-neighbor random hopping with no diagonal disorder leads to ordinary exponential $[\exp(-\lambda r)]$ localization. Numerical simulations show anomalous localization in dimensions 1 and 2, with additional periodic structure in some cases.

I. INTRODUCTION

We consider a disorder problem that is motivated by doped semiconductors, such as P-doped Si. In that system, the donor electrons are in Wannier orbitals centered on the randomly situated P atoms. The orbitals are connected by hopping matrix elements t_{ij} that vary exponentially with distance. The diagonal site energies ϵ_j are nearly constant. There is one electron per Wannier orbital, so that the Fermi level for the system is at the band center. (The electron-electron interaction, which is important in doped semiconductors, is not considered in this paper.)

In dimensions 1 and 2 (1D, 2D), almost any nonzero disorder causes exponential localization of all eigenfunctions, regardless of their energy.[1] The wave function decays from its maximum as $\exp(-\lambda r)$. An exception is that the band-center wave functions for some systems with pure off-diagonal disorder are not exponentially localized.[2] This paper extends previous results which will be cited in the text, (a) by proving a theorem about the eigenfunctions vanishing on one sublattice, (b) by extending a random walk argument in 1D (Ref. 2) to include first- and third-neighbor hopping, and (c) by demonstrating how bias can enter the random walk and result in exponential localization. We also find short-distance periodic correlations in wave functions that show random walk or biased random walk behavior at large distances. A numerical example with both first- and second-neighbor hopping is shown to have exponentially localized eigenstates. This demonstrates that there is no important distinction between diagonal and off-diagonal disorder, but only between bipartite and nonbipartite lattices. A lattice is bipartite if it consists of two sublattices A and B, with nonzero hopping only between A sites and B sites. Ziman has also pointed out that anomalous localization for off-diagonal disorder depends on the system being bipartite.[3] Oppermann and Wegner found that in a $1/N$ expansion, there is singular behavior in the density of states at $E=0$ for a bipartite lattice.[4]

Finally, we give numerical results for 2D systems.

A tight-binding model with disorder is described by the Hamiltonian

$$H=\sum_j \epsilon_j c_j^\dagger c_j+\sum_{jk} t_{jk} c_j^\dagger c_k, \tag{1}$$

where ϵ_j and t_{jk} are uncorrelated real random variables and $t_{jk}=t_{kj}$. We mainly consider off-diagonal disorder for which the ϵ_j are constant, taken to be zero. The band-center eigenstates then have energy zero. Some generalizations to include diagonal disorder and nonbipartite lattices are also considered. We further consider generalizations with t_{jk} complex and $t_{kj}=t_{jk}^*$, which allows uniform and random magnetic fields. Note that the diagonal disorder term ϵ_j could equally well be written as a hopping term t_{jj} that connects a site to itself. Thus a system with diagonal disorder cannot be bipartite.

This paper is organized as follows. Section II gives exact and analytic results: Section II A demonstrates that there are zero-energy eigenfunction(s) with vanishing amplitude on one sublattice for regular and irregular bipartite lattices in any dimension. Some generalizations to nonbipartite systems are included. Section II B gives analytic results for the random walk behavior of $\ln|\psi_j|$ for 1D systems with random first-neighbor hopping and for systems with random first- and third-neighbor hopping. Section II C shows how weak diagonal disorder leads to a *biased* random walk. In Sec. II D we discuss the density of states for the anomalously localized case.

Section III contains numerical results: Section III A gives results for 1D systems with first- and third-neighbor coupling, and also for systems with first- and second-neighbor coupling. The latter is *not* bipartite, and has ordinary exponential localization. The numerical stud-

ies find short-distance periodic behavior in addition to the long-distance random walk or exponential behavior. Section III B gives results for a 2D system and comparison with earlier work is made. Section IV contains a summary and a conclusion.

II. EXACT AND ANALYTIC RESULTS

A. Zeros of eigenfunctions

A bipartite lattice contains two sublattices A and B, with t_{jk}'s connecting sites on one sublattice only to sites on the other. Consider a finite system with n_A sites on the A sublattice and n_B sites on the B sublattice, with labels chosen so that $n_A \leq n_B$. The following theorem applies to the zero-energy eigenfunctions:

On any bipartite lattice with only off-diagonal disorder, there are at least $n_B - n_A$ linearly independent eigenfunctions with eigenvalue $E = 0$ and all amplitudes ψ_j equal to zero on the sites of the A sublattice.

Proof: The Schrödinger equation on site j for a zero energy eigenfunction is

$$E\psi_j = 0 = \epsilon_j \psi_j + \sum_k t_{jk}\psi_k. \tag{2}$$

Consider a bipartite lattice with all $\epsilon_j = 0$ and seek solutions with all ψ_j equal to zero on the A sublattice. The Schrödinger equation is trivially satisfied when j is on the B sublattice, because all ψ_k in the sum are zero. The Schrödinger equation is nontrivial when j is on the A sublattice, which gives n_A linear homogeneous equations. There are n_B unknowns, which are the nonzero ψ_j on the B sublattice. For $n_B > n_A$, there exist $n_B - n_A$ linearly independent solutions to the system of equations. (If the system of equations is singular, there will be more than $n_B - n_A$ solutions.)

Generalizations: Since all ψ_j are zero on the A sublattice anyway, nothing is changed at $E = 0$ by adding arbitrary off-diagonal or diagonal ($\epsilon_j \neq 0$) connections between A sublattice sites. If there are m B sublattice sites with connections to other B sites or nonzero diagonal terms, there are least $n_B - n_A - m$ linearly independent solutions with $\psi_j = 0$ on the A sublattice and on the m B sublattice sites. This last assertion has content only if $n_B - n_A - m > 0$.

The theorem applies in any dimension to lattices which may be any size and need not be regular (see Fig. 1). The fact that the theorem applies to irregular lattices is not surprising; since the t_{jk} can be arbitrary, parts of the lattice can be disconnected by setting some of the $t_{jk} = 0$, and any irregular lattice can be formed from a regular one in higher dimensions by selectively setting some hopping matrix elements to zero. The t_{jk} may have random sign or even be complex with $t_{kj} = t_{jk}^*$. Complex hopping allows an arbitrary magnetic field to be added to the system. Note that if $n_A = n_B$, there are typically no zero-energy eigenfunctions. Thus the 5×5 square lattice of Fig. 1(a) always has a zero-energy eigenfunction, but a 6×6 lattice typically does not. In addition to the above proof, these assertions have been verified numerically.

The zero-energy eigenfunctions described by the theorem are in the center of the band, where the center is determined either by counting eigenstates from the bottom, or from the average of the eigenvalues $\bar{E} = \sum_j E_j/N$, which is zero since the initial Hamiltonian is traceless. Under the generalizations that allow diagonal and off-diagonal disorder on the A sublattice, the zero-energy

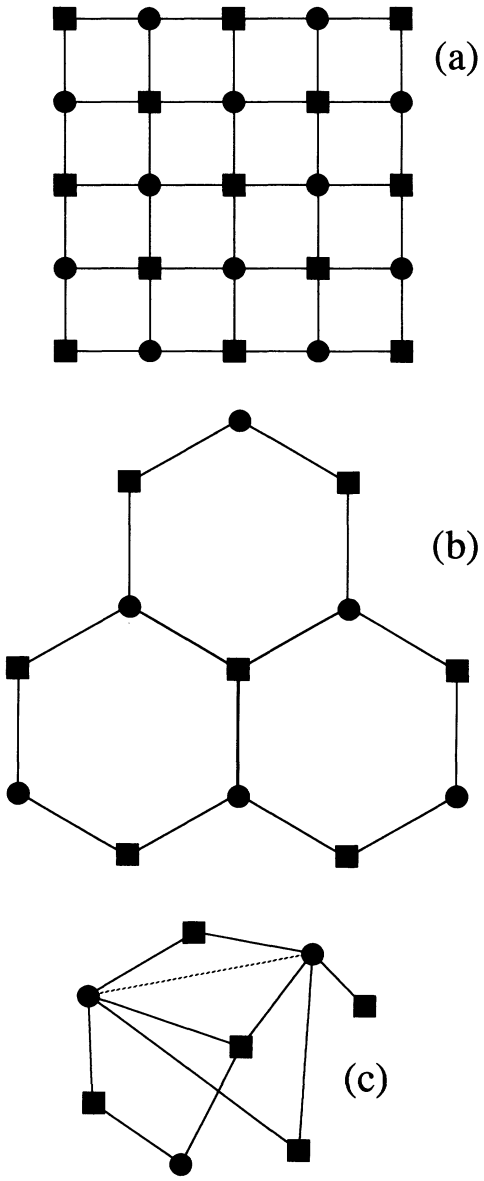

FIG. 1. Bipartite lattices with the A sublattice marked by circles, and the B sublattice marked by squares. Nonzero random hopping matrix elements are shown by solid lines. Both (a) and (b) have $n_B = n_A + 1$, and each have one eigenfunction with E=0, which has amplitude zero on the A sublattice (circles). (c) An irregular bipartite lattice, with $n_B = n_A + 2$, and hence with two independent $E = 0$ eigenfunctions, each of which has amplitude zero on the A sublattice. If a nonzero hopping matrix element is added on the striped bond, the lattice is no longer bipartite, but it still has two zero energy eigenfunctions with amplitude zero on the A sublattice.

eigenstates need not be at $\bar{E}$, but they are apparently always at the band center by counting eigenstates. The only justification we offer for the last assertion is that one can continuously turn on the A-A hopping and A diagonal disorder without in general causing any level crossings. These counting assertions have also been verified numerically.

The zero-energy eigenfunctions with zero amplitude on the A sublattice have unusual correlation functions in all the cases we have investigated. We speculate that the correlation functions are anomalous in general.

Since these results apply for arbitrary complex $t_{kj} = t_{jk}^*$, they are relevant to the problem of quantum localization in a random magnetic field, which has received much attention recently.[5] Note that if one is interested in the continuum problem, discretization on a square lattice results in completely different localization properties at the band center than discretization on a triangular lattice. (The triangular lattice is nonbipartite.) The above results also apply to the quantum percolation problem, in which some of the t_{kj} are set to zero with probability p.[6]

B. Off-diagonal disorder, $d = 1$

We first consider a 1D chain with nearest-neighbor hopping of random strength. To avoid spurious problems of disconnecting the lattice, we do not consider distributions in which t_{ij} assumes values close to 0 or ∞. Equation (2) becomes

$$t_{j,j-1}\psi_{j-1} + t_{j,j+1}\psi_{j+1} = 0. \tag{3}$$

On alternate sites (the B sublattice), the logarithm of the absolute value of ψ obeys the recursion relation

$$\ln|\psi_{j+1}| = \ln|\psi_{j-1}| + [\ln|t_{j,j-1}| - \ln|t_{j,j+1}|]. \tag{4}$$

The term in brackets is a random variable with zero mean and finite variance since random variables with different alternate site index j are uncorrelated. Thus, the quantity $\ln|\psi_{j+1}|$ on alternate sites undergoes a random walk, and a typical wave function decays like $\exp(-\lambda\sqrt{r})$ from its maximum, which is much slower than the usual $\exp(-\lambda r)$ decay found for diagonal disorder or off-diagonal disorder far from the band center. This random walk argument was first made by Fleishman and Licciardello.[2] Away from the band center the correlations should cross over to simple exponential at a length scale larger than ξ, where ξ diverges as $E \to 0$. Thus, although a finite 1D lattice with an even number of sites does not have an $E = 0$ eigenfunction, the eigenfunction with the smallest $|E|$ is expected to decay like $\exp(-\lambda\sqrt{r})$ for distances r essentially as large as the system size L.

To investigate whether the eigenstates described by the theorem generically have anomalous correlations, we also considered a 1D lattice with first- and third-neighbor random hopping, which leaves the lattice bipartite. At $E = 0$, the Schrödinger equation can be written

$$t_{j,j+3}\psi_{j+3} + t_{j,j+1}\psi_{j+1} + t_{j,j-1}\psi_{j-1} + t_{j,j-3}\psi_{j-3} = 0. \tag{5}$$

The eigenfunction is zero on the A sublattice which has j = odd. Numerical simulations of Eq. (5) indicate that at long distances, $\ln|\psi_j|$ undergoes a random walk (see Sec. III A). (It is interesting, however, that in short distances, a random walk was not observed.) This is not so simple to demonstrate analytically as it was for Eq. (3). One reason is that there is only one solution of Eq. (3), whereas there are three independent solutions of Eq. (5). A typical solution of Eq. (5) results in ordinary exponential growth or decay of the wave function, and also fails to satisfy the boundary conditions. It is only the particular solution that satisfies the boundary conditions that results in long-distance random walk behavior for $\ln|\psi_j|$.

We have made analytic progress with Eq. (5) only for the case where very dilute random impurities leading to off-diagonal disorder are present in an otherwise ordered lattice. (The general case is considered numerically in Sec. III A.) In the ordered part of the lattice, $t_{j,j\pm1} = t$ and $t_{j,j\pm3} = t'$, with $\tau \equiv t'/t$. We calculate the transfer matrix for an isolated impurity at site M so that the connected bonds $t_{M,M\pm1}$ and $t_{M,M\pm3}$ are random. In the ordered part of the lattice, there are three solutions for a given sublattice. One solution is always of the form $\psi_j = \cos(\frac{\pi}{2}j)$. For $-1 < \tau < 1/3$, there is in addition a pair of exponentially growing and decreasing solutions, ψ_+ and ψ_-. For τ outside that range, there is instead a pair of propagating solutions. Our analytic treatment applies only to the former case. For the exponential case with very dilute impurities, the appropriate solution is of the form $\psi_j = A_L\cos[\frac{\pi}{2}(j-M-1)] + B_L\psi_+$ to the left of site M, and $\psi_j = A_R\cos[\frac{\pi}{2}(j-M-1)] + B_R\psi_-$ to the right. By eliminating B_L and B_R we find

$$\ln|A_R| = \ln|A_L| + [\ln|R_1| - \ln|R_2|], \tag{6}$$

where

$$\begin{aligned} R_1 &= \alpha^2 t_{M,M+3} + \alpha t_{M,M+1} + t_{M,M-1} \\ &\quad + (\alpha^2 + \alpha - 1)t_{M,M-3}, \\ R_2 &= \alpha^2 t_{M,M-3} + \alpha t_{M,M-1} + t_{M,M+1} \\ &\quad + (\alpha^2 + \alpha - 1)t_{M,M+3}, \end{aligned} \tag{7}$$

and

$$\alpha = \frac{1}{2\tau}[\tau - 1 + \sqrt{(1+\tau)(1-3\tau)}\,], \tag{8}$$

where $\alpha = \psi_{j+2}/\psi_j$ for the exponentially decreasing solution. We assume that both nearest-neighbor bonds $t_{M,M\pm1}$ have the same probability distribution p_1, and both third-neighbor bonds $t_{M,M\pm3}$ have the same distribution p_3. Then R_1 and R_2 are random numbers with the same probability distribution, and the logarithmic amplitude again undergoes an unbiased random walk after multiple impurity sites, resulting in an eigenfunction with $\exp(-\lambda\sqrt{r})$ decay from its maximum.

Equation (7) is for the case where the site M is on the sublattice on which the wave function vanishes. If the site M is on the other sublattice, the equations for R_1 and R_2 are interchanged, and the conclusion about the unbi-

ased random walk is unaffected. As shown below, there is numerical evidence that the logarithmic amplitude undergoes a random walk at long distances even when the assumptions about dilute impurities and the magnitude range of τ are relaxed. We have not, however, demonstrated this analytically.

C. Diagonal disorder, $d = 1$

We propose that at least in 1D, the localization problem is always a random walk. The usual exponentially localized cases are random walks *with bias*. In the special cases that have anomalous localization, the bias disappears. We consider a problem in which the bias can be increased continuously from zero by adding a small amount of diagonal disorder. Let ϵ_j be the diagonal energy of site j. We consider here only nearest-neighbor hopping with t_j the hopping amplitude from site j to $j+1$. Using the Schrödinger equation, the transfer matrix $\mathcal{M}$ to propagate the $E = 0$ wave function by two sites is given by

$$\begin{bmatrix} \psi_{j+2} \\ \psi_{j+1} \end{bmatrix} = \begin{bmatrix} \frac{\epsilon_j \epsilon_{j+1}}{t_j t_{j+1}} - \frac{t_j}{t_{j+1}} & \frac{\epsilon_{j+1} t_{j-1}}{t_j t_{j+1}} \\ -\frac{\epsilon_j}{t_j} & -\frac{t_{j-1}}{t_j} \end{bmatrix} \begin{bmatrix} \psi_j \\ \psi_{j-1} \end{bmatrix}. \tag{9}$$

Consider first the case where there is off-diagonal but no diagonal disorder, so that all $\epsilon_j = 0$. Then the only terms remaining in Eq. (9) are on the diagonal. The matrix $\mathcal{M}_n$ to transfer the wave function n sites (n even) is

$$(\mathcal{M}_n)_{1,1} = \frac{t_{j+n-2}}{t_{j+n-1}} \cdots \frac{t_{j+4}}{t_{j+5}} \frac{t_{j+2}}{t_{j+3}} \frac{t_j}{t_{j+1}}, \tag{10}$$

$$(\mathcal{M}_n)_{2,2} = \frac{t_{j+n-3}}{t_{j+n-2}} \cdots \frac{t_{j+3}}{t_{j+4}} \frac{t_{j+1}}{t_{j+2}} \frac{t_{j-1}}{t_j}, \tag{11}$$

with zero off-diagonal elements. The logarithm of the wave function on the even sublattice is executing a random walk. It can be seen that aside from "end effects," $(\mathcal{M}_n)_{2,2}$ is the inverse of $(\mathcal{M}_n)_{1,1}$, so that the odd sublattice is not executing an independent random walk, but rather the mirror image of the even sublattice walk.

Now add very dilute diagonal impurities ϵ_j, with ϵ_j comparable in magnitude to the t_j. The impurities occur with a density $1/L$, where L is a distance long enough that $\ln|\psi|$ has diffused more than one unit (increasing on one sublattice, decreasing on the other). Because $\epsilon_j \neq 0$, the transfer matrix, Eq. (9), now has one nonzero off-diagonal matrix element. The diagonal disorder mixes the even and odd sublattice amplitudes. When two numbers ψ_j and ψ_{j-1} that differ by orders of magnitude are added together, the magnitude of the sum is approximately equal to the magnitude of the larger number. Thus, depending on the sublattice the impurity lands on, it has a 50% chance of doing essentially nothing (in the case that the impurity is on the sublattice with smaller $|\psi|$), and a 50% chance of resetting the smaller sublattice amplitude to a value comparable to the larger amplitude (in the opposite case). This process of taking the walks that have wandered in one direction (toward a smaller absolute value, call it "left") and replacing them by a displacement of equal magnitude to the opposite direction ("right") results in a biased random walk. The motion of $\ln|\psi_j|$ is hence drift plus diffusion. The diffusion constant is $D = \sigma^2/2$, where σ^2 is the variance of the random variable $\ln|t|$. The drift corresponds to exponential localization with a localization length (to within a factor of order unity) $\xi = \sqrt{L}/\sigma$. The drift can be made arbitrarily small compared to the diffusion.

D. Density of states

Thouless has shown that in 1D, the localization length is directly related to the density of states.[7] Thus since off-diagonal nearest-neighbor disorder in 1D has anomalous localization at $E = 0$, it also has a singular density of states at $E = 0$. This has been observed numerically.[8,9]

III. NUMERICAL RESULTS

In this section, we present the results of our numerical investigation of finite systems, which confirm and extend the above ideas. We first discuss the one-dimensional system with only first- and third-neighbor hopping, and contrast this with the case of first- and second-neighbor hopping. Then we study two-dimensional systems and show that while the localization properties are still anomalous, there are important differences from the one-dimensional cases.

A. One-dimensional systems

First, we summarize the general technique we used to study 1D systems. We consider only finite-range hopping, so that $t_{ij} = 0$ if $|i-j| > l$. The bipartite property requires that $t_{ij} = 0$ for $|i-j|$ even. The Schrödinger equation on site j, Eq. (2), is a relation between $2l+1$ amplitudes,

$$\psi_{j+l} = \sum_{k=1}^{2l} \tau_k^{(j)} \psi_{j-l-1+k},$$

where

$$\tau_k^{(j)} = -\left[t_{j,j-l-1+k} + \delta_{k,l+1}(\epsilon_j - E) \right] / t_{j,j+l}.$$

Thus one can construct recursion relations among the vectors defined as $\Psi_n = (\psi_{n+2l}, \cdots, \psi_{n+1}, \psi_n)^T$ (T denotes transpose):

$$\Psi_{n+1} = M_n \Psi_n, \tag{12}$$

where M_n is a $2l \times 2l$ matrix whose elements are given by $(M_n)_{1,j} = \tau_{2l+1-j}^{(n+l)}$, $(M_n)_{i,j} = \delta_{i+1,j}$ $(i \neq 1)$. From this, we have

$$\Psi_{n+1} = M_n \cdots M_2 M_1 \Psi_1 \equiv \mathcal{M}_n \Psi_1.$$

One can solve this linear equation for the vector Ψ_1 so that the system satisfies the boundary conditions at both ends. Once Ψ_1 is obtained this way, Eq. (12) is used to

generate the entire wave function. A special case of $\mathcal{M}_2$ is given in Eq. (9). Note that a system that is not strictly one dimensional (i.e., strips) can also be studied similarly with a straightforward generalization. A more standard method to extract the localization length is to find the eigenvalue of $\mathcal{M}_n$ for large n that is closest to unity.[10]

The alternate method we used generates the explicit wave function that satisfies the boundary conditions, including the zeros on one sublattice and the short-distance periodic correlations.

By computing the appropriate correlation functions for different realizations of disorder and then taking their average, one can study the behavior of this system. We define two types of correlation functions:

$$g_1(r) = \left\langle \left| \ln|\psi_j| - \ln|\psi_{j+r}| \right| \right\rangle' ,$$
$$g_2(r) = \left\langle \ln|\psi_{j_{\max}}| - \ln|\psi_{j_{\max}\pm r}| \right\rangle , \tag{13}$$

where $\langle\cdots\rangle$ indicates averaging over different realizations and $\langle\cdots\rangle'$ is the average over different "starting" sites j as well as over different realizations. We have denoted by $j_{\max}$ that site with the largest amplitude $|\psi_j|$. For bipartite lattices, the functions g_1 and g_2 are plotted only for the sublattice with nonzero ψ_j. In the case of one-dimensional problems that exhibit random-walk-like behavior, both of these functions numerically show $g(r) \sim \sqrt{r}$ at large distances.

The 1D system with first- and third-neighbor random hopping is studied in this manner. We are interested in the $E = 0$ state when the on-site energies $\epsilon_j = 0$. Since in this state all the amplitudes on the sites of the even sublattice are zero, Eq. (12) reduces to a recursion with 3×3 matrices rather than 6×6.

The resulting correlation function g_1 is shown in Fig. 2. In the figure, $(g_1)^2$ is plotted against r so that $g_1 \sim \sqrt{r}$ will appear linear. This system shows a linear behavior which is similar to that of the case with only nearest-neighbor couplings. (The correlation function g_2, which is not shown, is similar.) The interesting period-8 oscillations can be explained as follows: Recall that in the previous section, we considered the case where $t_{j,j+1}$ and $t_{j,j+3}$ are fixed numbers rather than random variables. For $\tau \equiv t_{j,j+3}/t_{j,j+1}$ outside the interval $[-1, 1/3]$, there is a solution of the form $\psi_j = \cos(qj + \phi)$ with

$$q = \frac{1}{2}\cos^{-1}\left(\frac{\tau - 1}{2\tau}\right) , \tag{14}$$

in addition to a solution of the form $\psi_j = \cos(\frac{\pi}{2}j + \phi)$. In the disordered case, τ is taken equal to $\langle t_{j,j+3}\rangle/\langle t_{j,j+1}\rangle$. We have checked numerically for several cases that the wavelength $\tilde{\lambda}$ (= 8 in Fig. 2) of the short-distance oscillations in g_1 is given by the interference of the $k = \pi/2$ and the $k = q$ wave functions, with $\tilde{\lambda} = 2\pi/(\frac{\pi}{2} - q)$. In other words, with the level of disorder we have used, the

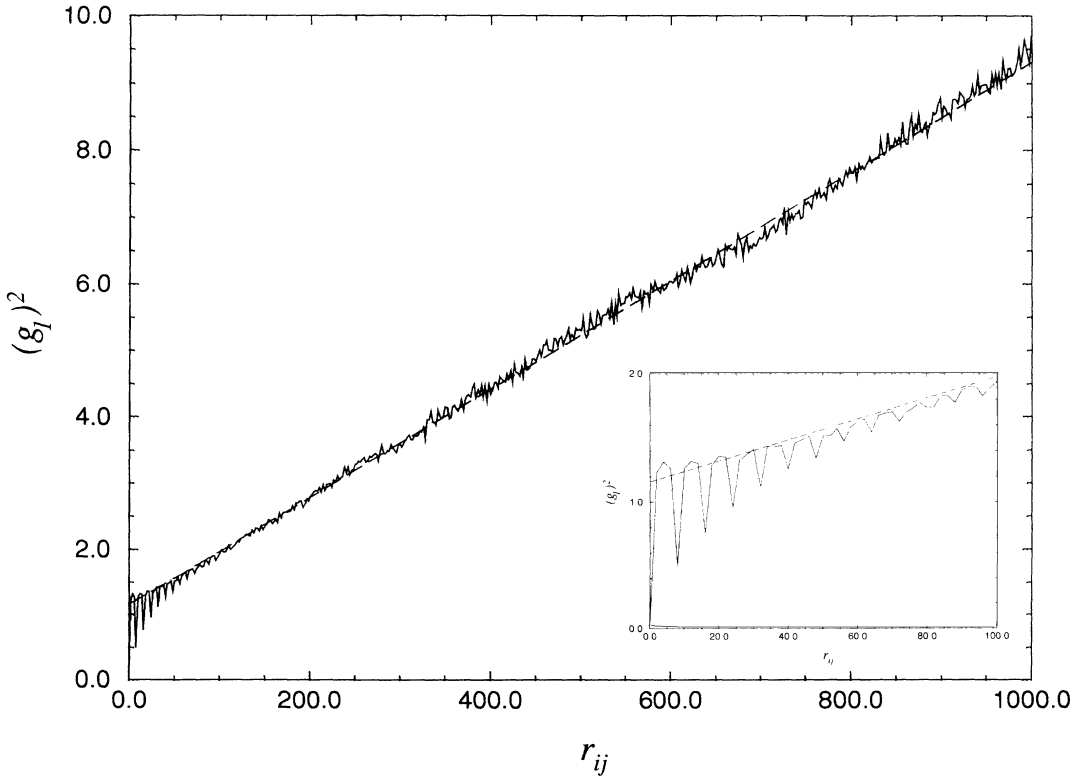

FIG. 2. The *square* of the correlation function g_1 for 1D systems with random first- and third-nearest-neighbor hopping, obtained by averaging over 10 000 realizations. Both the first- and third-neighbor couplings are random variables that are uniform in the interval [0.15, 1]. In order to eliminate the influence of the boundary effects, we have used the middle 1001 sites of 2001-site systems. The straight line fit is $(g_1)^2 = 1.1605 + 0.008\,148\,8r$. The inset shows the behavior near $r = 0$.

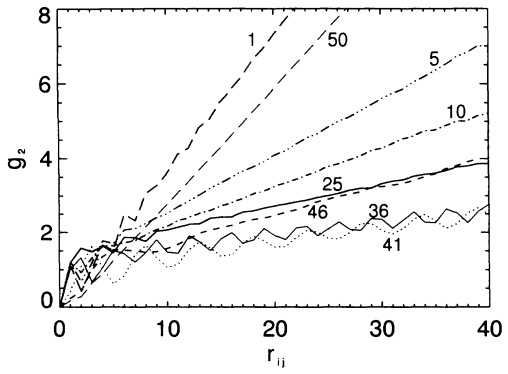

FIG. 3. The correlation function g_2 for 1D systems with random first- and second-neighbor hopping, obtained by averaging over 4000 realizations. Both the first- and second-neighbor couplings are random variables that are uniform in the interval [0.15, 1]. In contrast to Fig. 2, g to the first power is plotted so that a straight line implies ordinary exponential localization. Correlation functions are labeled from the lowest-energy (1) to the highest-energy (50) eigenfunction for the 50-site system.

eigenstate looks *locally* like a plane wave. The period of the oscillations can be varied by changing the random distributions. For the example of Fig. 2, $\tau = 1$, which results in the observed wavelength $\tilde{\lambda} = 8$.

Next we consider the case of first- and second-neighbor hopping, which does *not* leave the lattice bipartite. For this case the theorems do not apply, and there is in general no zero-energy eigenfunction. We exactly diagonalized 50-site chains and compiled statistics for all eigenfunctions (see Fig. 3). The figure shows that for all energies, g_2 increases linearly with r, indicating exponential localization $\psi \sim \exp(-\lambda r)$. There is no symmetry between the upper and lower band edges. For example, state 46, with the fifth highest energy, has a different λ than state 5, with the fifth lowest energy. In the region where λ is smallest (eigenstates 36–44), g_2 shows periodic oscillations superimposed on the linear growth. The period of the oscillations changes with the energy of the eigenstate. These periodic oscillations can again be explained by considering the problem with no disorder, with $t_1' = \langle t_1 \rangle$ and $t_2' = \langle t_2 \rangle$, resulting in a dispersion relation $\epsilon(k) = 2t_1' \cos(k) + 2t_2' \cos(2k)$. In the ordered case, the periodicity of $\cos(kr)$ with k chosen to correspond to the appropriate eigenstate is equal the observed periodicity in $g_2(r)$. For some values of ϵ, there are four allowed k's. The oscillations in Fig. 3, however, are in a region where there are only the usual two allowed k's.

B. Two-dimensional systems

In view of the unusual property of the $E = 0$ state of systems in 1D, we investigated 2D systems numerically in order to determine how dimensionality affects the result. We studied square lattices with nearest neighbor hopping and only off-diagonal disorder.

In 2D, the simple Lanczos method was used to find the lowest eigenstate of the matrix H^2 where H is the Hamiltonian matrix for a system with odd number of sites. Since it is already known that there is an $E = 0$ state for H, the lowest-energy eigenstate of H^2 has eigenvalue 0 and an eigenvector that coincides with that of H. Statistical errors were estimated by averaging over a number of realizations (typically 50–200). To assess the localization properties of the wave function, the correlation function g_2 of Eq. (13) was computed. Exponentially localized states show a linear relationship between g_2 and r. The function g_1 that involves all site pairs is not convenient in 2D in that it does not have this property.

The result for 75×75-site systems is shown in Figs. 4 and 5. It is clear that g_2 does not vary linearly with r so that the $E = 0$ state of this system is *not* exponentially localized. This state is less localized than the $E = 0$ state in 1D in the sense that $\langle |\psi_r/\psi_{j_{\max}}| \rangle$ decays slower than $\sim \exp(-\lambda\sqrt{r})$. We also note that the states away from $E = 0$ show standard $\sim \exp(-\lambda r)$ behavior. These states are not shown in the figures.

To better quantify the behavior of $g_2(r)$, we attempted to fit the following form to the numerical data, corresponding to $\langle |\psi_r/\psi_{j_{\max}}| \rangle \sim \exp(-Ar^\theta)$:

$$g_{\rm ex}(r) = Ar^\theta ; \tag{15}$$

as well as the form corresponding to power-law decay $\langle |\psi_r/\psi_{j_{\max}}| \rangle \sim r^{-\alpha}$:

$$g_{\rm PW}(r) = \alpha \ln r + B. \tag{16}$$

We also tried $\langle |\psi_r/\psi_{j_{\max}}| \rangle \sim \exp[-\gamma(\ln r)^{1/2}]$:

$$g_{\rm Z}(r) = \gamma\sqrt{\ln r} + C \tag{17}$$

following Ziman (see below). The best fits to the data shown in the figures are obtained at $(\theta, A) = (0.235, 2.36)$, $(\alpha, B) = (1.17, 1.34)$, and $(\gamma, C) = (3.79, -1.65)$. All of these functional forms are good fits

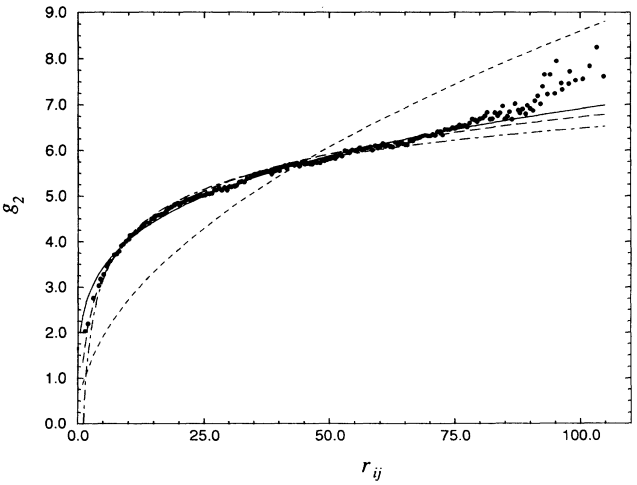

FIG. 4. The correlation function g_2 vs r for 2D systems. The solid curve shows the best fit with the form $g_2(r) = Ar^\theta$, the dashed line is with $g_2(r) = \alpha \ln r + B$, and the dot-dashed line is with $g_2(r) = \gamma\sqrt{\ln r} + C$. The curve with short dashes is the best fit with $g_2(r) = C\sqrt{r}$, corresponding to the dependence in the one-dimensional case.

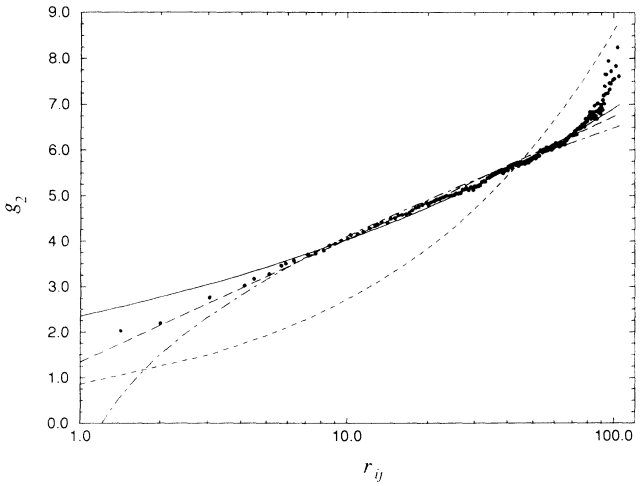

FIG. 5. The same as Fig. 4, but with r plotted on a logarithmic scale.

to the data, with the power law working better at short distances.

We point out that our numerical result is not sensitive to the size of the system investigated. The lattices with 21×21, 31×31, 41×41, and 51×51 showed essentially the same behavior. We cannot of course rule out different behavior at distances larger than those studied.

Soukoulis *et al.* have previously simulated the $E = 0$ localization problem in 2D with off-diagonal disorder.[11] They find that power-law localization $r^{-\alpha}$ fits their data, and that α changes continuously as the probability distribution for t is changed. They also find exponential localization for off-diagonal disorder on a triangular lattice, which is not bipartite. Ziman has proposed an approximate theory for localization by off-diagonal disorder that applies to any dimension.[3] In two dimensions, his approximation yields a functional form $\langle|\psi_r/\psi_{j_{\max}}|\rangle \sim \exp[-\gamma(\ln r)^{1/2}]$, which fits our data reasonably well. It would be interesting to check Ziman's prediction that states are extended in $d > 2$ with further numerical studies. Other work on off-diagonal disorder is contained in Refs. 12–17.

IV. SUMMARY AND CONCLUSION

We have shown that midband states of bipartite systems (and some generalizations) vanish on one sublattice. We believe that midband states on bipartite lattices are never exponentially localized. This hypothesis is supported by analytic and numerical results for 1D systems with nearest-neighbor, first- and second-neighbor, and first- and third-neighbor hopping, for 1D systems with diagonal disorder, and for 2D systems with nearest-neighbor hopping. The crucial property for anomalous localization is a bipartite lattice, not the presence of off-diagonal and absence of diagonal disorder. Diagonal disorder ϵ_j is identical to a connection of a site to itself (t_{jj}) and always destroys the bipartite nature of a lattice, whereas off-diagonal disorder may or may not destroy the bipartite nature of a lattice.

In one dimension, anomalous localization corresponds to an unbiased random walk, and ordinary localization to a biased random walk.

Finally, in connection with doped semiconductors, which are dominated by off-diagonal disorder, we conclude that localization should be of the ordinary exponential variety, because there is no reason that the t_{ij} should leave the lattice even approximately bipartite.

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