# Study of electronic states with off-diagonal disorder in two dimensions

C. M. Soukoulis, I. Webman, G. S. Grest, and E. N. Economou*
*Corporate Research Science Laboratories, Exxon Research & Engineering Co., Linden, New Jersey 07036*
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The nature of electronic states in a two-dimensional tight-binding model with off-diagonal disorder is examined by iterative methods applied to very long strips of finite width $M$. We find that for $E=0$ the localization length depends linearly on $M$ for all disorders $W$. This indicates a $R^{-\gamma(W)}$ behavior of the wave function, and provides a singular deviation from the belief based on scaling theory that all states are exponentially localized in two dimensions. However, for all $E\neq 0$, states are exponentially localized and scaling behavior is obeyed.

Recently, significant advances have been made[1,2] in understanding Anderson's localization in disordered systems. Much of the work has been based on the idea[3] that the extended or localized nature of the eigenstates can be determined by a single scaling variable, the dimensionless conductance $g(L)$ of a system of length $L$. By assuming that the quantity $\beta(g)\equiv d\ln g/d\ln L$, which describes the length dependence of $g$, is a monotonic and nonsingular function of $g$ only, one obtains that $g\rightarrow 0$ as $L\rightarrow\infty$ for any disordered system of dimensionality lower than or equal to 2.

Various numerical approaches such as the direct determination of the eigenfunctions,[4] sensitivity to boundary conditions,[3] calculation of the transmission coefficient,[5] evaluation of the conductivity,[6] recursion methods,[7,8] localization function method,[9] etc.[10] have been used to test these ideas. The predictions of the numerical studies in 2D (two dimensions) range from the existence of an Anderson transition[4,6] to localization for any amount of disorder.[5,8,9] Most of the numerical calculations and especially the very recent work,[5,8] support the predictions of the scaling theory for 2D; that is, all states are exponentially localized for any amount of disorder.

These numerical studies were performed for a tight-binding model defined by the Hamiltonian

$$H=\sum_n \epsilon_n \,|n\rangle\langle n| + \sum_{n,m}{}' V_{nm}\, |n\rangle\langle m| \ ,$$

with only diagonal disorder, i.e., the diagonal matrix elements $\epsilon_n$ are random variables. The role of randomness in the off-diagonal matrix elements $V_{nm}$ has not been studied extensively until recently,[11–13] since it was presumed that off-diagonal disorder is very similar to the diagonal one. A 1D system with only off-diagonal disorder provided the first indication that this may not be so. At the center of the band[12,13] of this system, the wave function decays not exponentially with the distance $L$ but more slowly as $\exp(-\alpha\sqrt{L})$.

It is the purpose of this paper to examine the nature of the eigenstates in a 2D square lattice with only off-diagonal disorder by using recently improved iterative methods[7,8] applied to very long strips of finite width. The present work is a test of how sensitive, if at all, the scaling theory[1] is to different types of disorder. Our numerical results show that at the center of the band the localization length depends linearly on the strip width for all values of the off-diagonal disorder. This indicates a power-law type behavior of the wave function. This result is in contrast with the case of diagonal disorder in 2D where numerical studies[5,8] show that at $E=0$ even for low disorder the states are exponetially localized as predicted by scaling theory.[1] However, we find that for $E\neq 0$ the states are exponentially localized and the localization length obeys finite size scaling behavior consistent with the ideas of scaling theory of Abrahams *et al.*

We considered a system of length $N\rightarrow\infty$ in the $x$ direction and length $M$ in the $y$ direction described by the usual Anderson tight-binding Hamiltonian with constant diagonal matrix elements. The off-diagonal matrix elements $V_{nm}$ for nearest neighbors are random variables and zero otherwise. We use a rectangular probability distribution of width $W$ for the logarithm of the $V_{nm}$,

$$P(\ln V_{nm}/V_0)=\begin{cases} 1/W & \text{if } |\ln V_{nm}/V_0|\leq W/2 \\ 0 & \text{otherwise} \ , \end{cases} \tag{1}$$

where $V_0=1$ is taken as the unit of energy. $W$ is a good measure of the strength of the off-diagonal disorder.[12] Periodic boundary conditions are imposed on the $y$ direction. For $N \gg M$ the system is one dimensional and therefore we can define a localization length $\lambda$ for a given energy $E$ disorder $W$ and width $M$. By studying $\lambda$ vs $M$ for given $E$ and $W$, one can predict the behavior of the 2D system ($M \to \infty$). We used two independent numerical methods for calculating $\lambda$. In the first method, the matrix element $\langle 1 \mid G(N) \mid N \rangle$ of the Green's function between states located at the first and $N$th columns of the strip is found by iterating the following equations:

$$A_n^{-1} = A_{N-1}^{-1} V_{N-1,N} B_N \; , \tag{2}$$

$$B_N = (E - H_N - V_{N,N-1} B_{N-1} V_{N-1,N})^{-1} \; . \tag{3}$$

Here $A_N^{-1} = \langle 1 \mid G(N) \mid N \rangle$, $B_N = \langle N \mid G(N) \mid N \rangle$, and $H_N$ is the Hamiltonian of the $N$-column system. The localization length $\lambda$ is now given by

$$\lambda = \lim_{N \to \infty} [2(N-1)^{-1} \ln \mathrm{Tr} \mid \langle 1 \mid G(N) \mid N \rangle \mid^2 \; . \tag{4}$$

By iterating Eqs. (2) and (3) in the above manner, only the largest eigenvalue of $A_N^{-1}$, which is related to the localization length, contributes to Eq. (4). We can also combine Eqs. (2) and (3) into a single equation for $A_N$, as first noted by MacKinnon and Kramer. The second method we employed is based on the multiplicative ergodic theorems[14–16] for products of random matrices. The amplitudes of the wave function at the $i$th and $(i+1)$th columns are related to the amplitudes on the $i-1$ and $i$th column by the relation

$$\begin{bmatrix} \alpha_{i+1} \\ \alpha_i \end{bmatrix} = \hat{T}_i \begin{bmatrix} \alpha_i \\ \alpha_{i-1} \end{bmatrix} , \tag{5}$$

where $\hat{T}_i$ are $2M \times 2M$ matrices whose elements depend on the values of the random off-diagonal matrix elements of $H_i$. The localization length $\lambda$ is related to the eigenvalues of the matrix $\hat{T}$ defined by the limit[15]

$$\lim_{N \to \infty} \prod_{i=1}^{N} \hat{T}_i / \hat{T}^N = \hat{1} \; . \tag{6}$$

$\lambda$ is now given by

$$\lambda^{-1} = \mid \ln(\min\{ \mid \Gamma_k \mid \}) \mid \; ,$$

where $\{\Gamma_k\}, k = 1, 2M$ are the eigenvalues of $\hat{T}$. The details of the two methods which are a generalization of the recent recursive methods[7,8] to include off-diagonal disorder can be found in Refs. 7 and 8. These two methods contain no restriction on the size of the system other than the computer time available. Therefore, one can increase $N$ until a given accuracy of the localization length is obtained. Typically we iterated the solution until $\Delta\lambda/\lambda \simeq 2\%$, where $\Delta\lambda$ is the standard deviation of $\lambda$. For off-diagonal disorder of $W=2$ and width $M=31$, $N$ was run for $10^5$ sites; for larger disorder and smaller $M$ the convergence is faster. In general, we found that the transfer matrix technique was significantly faster than the Green's-function recursion method and within statistical error, we obtained the same results by the two methods. We want to mention that all these recursive methods cannot reliably calculate the length dependence of the dc conductivity $\sigma$ using the Kubo-Greenwood formula. Even in 1D, where we know that all states are exponentially localized, the Kubo-Greenwood formula for $\sigma$ has problems.[17] Therefore, by calculating $\lambda$ in 2D and then trying to obtain the scaling function $\beta(g)$ from $\lambda$ one has to introduce another possible approximation relating $\sigma$ to $\lambda$.[8]

We calculate the localization length $\lambda(E,W,M)$ for $d=2$ with $2 \le W \le 16$ for both $E=0$ and $E \ne 0$ and for a number of different values of $M$. In Fig. 1 we plot $\lambda_M$ as a function of $M$ for different $W$'s at the center of the band ($E=0$). Figure 1(a) shows our results for $M$ even and Fig. 1(b) for $M$ odd.[18] Note that $\lambda_M$ increases almost linearly with $M$ for all $W$'s even for very large disorders. This indicates that we cannot define a finite localization length for the infinite lattice. Therefore, following the arguments of Ref. 7, we propose that for a 2D lattice at the center of the band with only off-diagonal disorder, the wave function falls off with distances as $R^{-\gamma(W)}$, which suggests a very weakly localized or very weakly extended behavior depending on the value of $\gamma$. In Fig. 2 we plot the exponent $\gamma$ as a function of $W$, taken from the case of even or odd $M$. The exponent $\gamma(W) = 1/\pi b(W)$, where $b(W) = \lambda_M / M$. Note that $\gamma$ increases linearly with $W$, and is larger than one when $W=11$. Therefore, for $W \le 11$, the states are weakly extended. Next we examined whether or not this "power-law localization" persists for $E \ne 0$. As shown in Fig. 3, $\lambda_M$ is no longer linear in $M$, but it approaches a finite limit as $M \to \infty$, which is the localization length. Thus the power-law localization is an exception appearing only for $E=0$ and for the case of off-diagonal disorder. It is tempting to attribute this exception to the possible existence in a square lattice of a logarithmic singularity in the density of states $N(E)$ at $E=0$

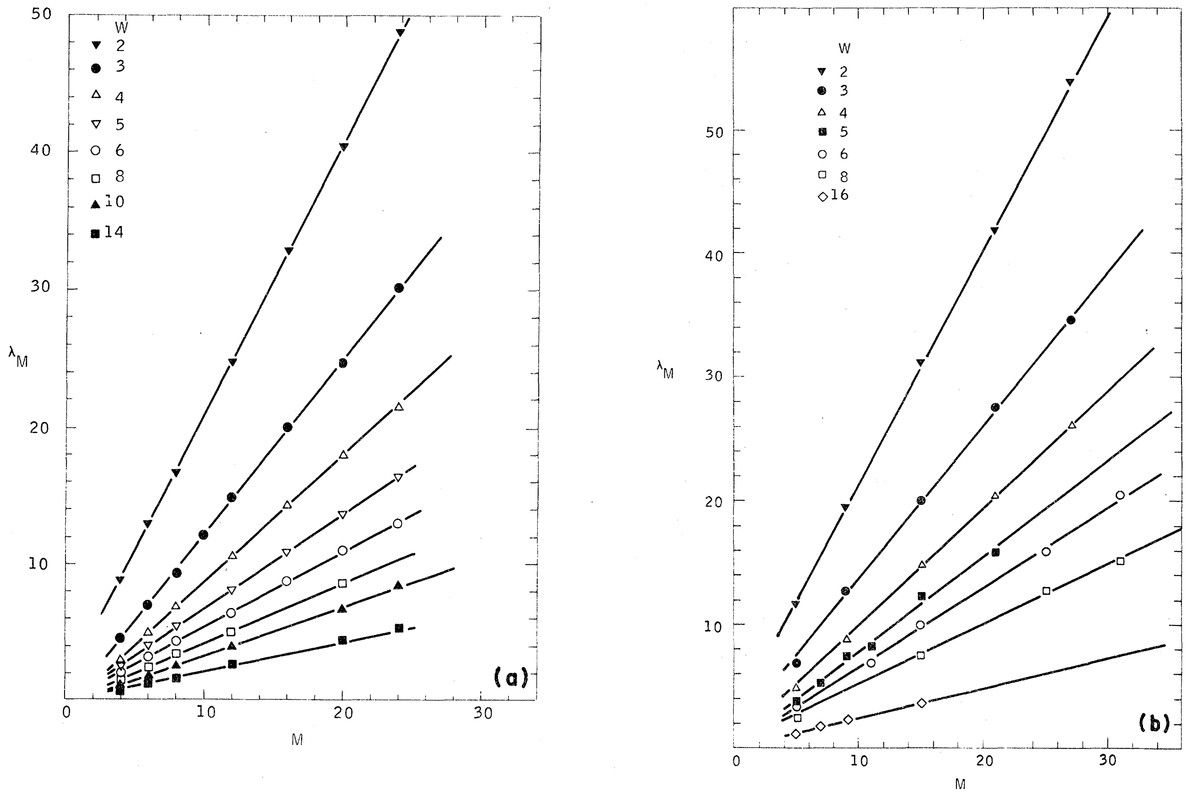


FIG. 1. Localization length $\lambda_M$ vs the width $M$ for even (a) and odd (b) strips.

even in the presence of off diagonal disorder. To further check this idea, we calculated $\lambda$ vs $M$ at $E=0$ and $W=10$ for a triangular lattice, which does not have any singularity in $N(E)$ at $E=0$; we found that the states are exponentially localized. We also checked, for the triangular lattice and for $W \neq 0$, the case $E=-2$ [where at zero disorder $N(E)$ is singular] and we found exponentially localized states. Therefore, we tentatively conclude that this power-law localization for off-diagonal disorder at $E=0$ for a square lattice is due to the logarithmic singularity at $N(E)$, which seems to persist even for $W \neq 0$.

Our results for large $E(\gtrsim 10^{-2})$ and large $M$ obey the scaling law

$$\lambda_M/M = f(\lambda_\infty/M) \tag{7}$$

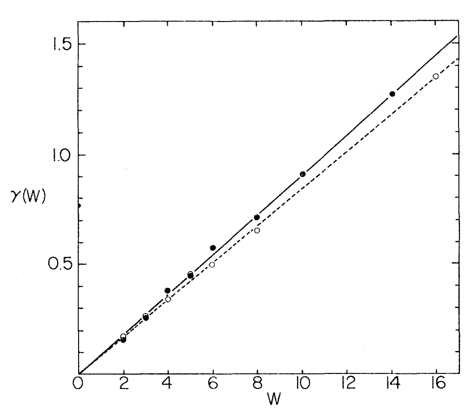


FIG. 2. Exponent $\gamma(W)$ vs $W$ for only off-diagonal disorder at $E=0$ for $M$ odd (open circles) and $M$ even (closed circles).

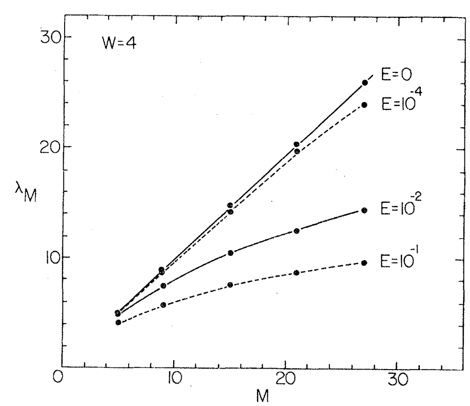


FIG. 3. $\lambda_M$ vs $M$ for four different energies $E$ with $W=4$.

found by MacKinnon and Kramer; this is consistent with the idea of one-parameter scaling. On the other hand, the case of $E=10^{-4}$ shown in Fig. 3 is so close to the $E=0$ power-law localization that one probably needs to reach $M$'s much larger than $M=31$ in order to see the scaling behavior. To further check the universality of the scaling behavior, we have examined some cases with only diagonal disorder and $E\neq 0$; we found that data fall on the same scaling function as in Eq. (7).

Our present results provide further support to the idea that the one-parameter scaling hypothesis (which leads to exponential localization for $d\leq 2$) is true in a generic sense. On the other hand, the present work clearly demonstrates that exceptions to the rule for exponential localization for $d\leq 2$ do exist.

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*Permanent address: Department of Physics, University of Crete, Iraklion, Crete, Greece.

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[18]In both methods the values of $\lambda$ at $E=0$ for strips of even number of lines are lower by $\sim 10\%$ than the corresponding values for odd number of rows. Examination of the behavior for strips with open boundary conditions rather than periodic ones by both numerical and analytical methods shows that odd strips at $E=0$ behave similarly to one-dimensional systems with purely off-diagonal disorder, namely the states are localized more weakly than exponential. The introduction of periodic boundary conditions amounts to connecting many 1D channels in parallel which results in a reduction of the statistical fluctuation responsible for this anomalous localization and in recovering the exponential decay. We believe, however, that the slight difference between the values of $\lambda$ for even and odd strips with periodic boundary conditions is a remnant of the more drastic difference for the single channel case.