

Localized states in disordered systems

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Abstract. The Anderson problem of the localization of electrons in disordered systems is discussed by analysing the residues of the off diagonal propagator. On the assumption that the eigenvalues are statistically independent, Anderson's upper limit is reproduced, while improved conditions are obtained by assuming specific correlations amongst the levels. The form of the wavefunctions and analytical structure of the selfenergy are also discussed. Several types of disorder are analysed and mobility edges are shown to exist in some cases.

1. Introduction

The problem of localization in certain random lattices has recently been the subject of some controversy. Anderson (1958, 1970) introduced a simple model of cellular disorder in which he deduced that under certain conditions, the imaginary part of the selfenergy must be zero except on a discrete set of points. He therefore concluded that the wavefunctions for his model decay exponentially on the average away from the centre of localization. This work has been reviewed by Ziman (1969) and Thouless (1970). Halperin (1968) has shown that if the variance of the wavefunction is finite, then the residual conductivity is zero, whilst Mott (1967) has suggested that there exists a certain critical energy E_c separating localized and delocalized states. In this work the following aspects of the subject are discussed: (i) the existence of the localized regime; (ii) the properties of the wavefunction and selfenergy before and after the transition; (iii) the determination of the transition points E_c .

Our analysis of the Anderson model (§ 2) differs from previous discussions by concentrating on the off diagonal propagator, whose residue $R_{ij}(\mathcal{E}_\alpha)$ at the pole with energy \mathcal{E}_α represents a probability amplitude of a transition from site i to site j . This residue is effectively an order parameter for the phase transition from localized to delocalized states, and consequently it seems the natural object to study. R_{ij} has several advantages over the selfenergy of the diagonal Green function in that, for example, it is always bounded by unity, and has a direct interpretation in terms of the localized nature of the eigenfunctions. If states are localized, then the residue tends to zero exponentially as the distance between sites tends to infinity.

It is shown that R_{ij} can be written as a sum of products of the form

$$\prod_{k \neq \alpha}^N \frac{V}{|\mathcal{E}_\alpha - \mathcal{E}_k^{(N)}|} = \exp(S_{N-1}) \quad (1.1)$$

where $\mathcal{E}_k^{(N)}$ is the renormalized local energy and V the hopping potential. In the localized phase, the renormalized levels are shown to be approximately distributed with the density of eigenstates, and the upper limit of Anderson is reproduced under the assumption that the eigenvalues are independently distributed. However, this assumption leads to a long tail on the distribution of the residue which violates the condition that it is bounded by unity. To lessen the importance of the long tail, the distribution of $\ln |R_{ij}|$ is first approximated by a Gaussian and then by a Gaussian with a cut off. These distributions lead to

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new estimates of the critical values of the parameter governing the transition, and are compared with a lower limit based on percolation theory. In §3, the variance of the wavefunction for a linear chain is shown to be infinite in the delocalized region and finite otherwise.

The form of the selfenergy before and after the transition has led to some confusion, and in §4 we show that on the delocalized side, its imaginary part is not zero everywhere, whereas on the localized side it is zero except at a discrete set of points. This is in agreement with Anderson (1970). The average selfenergy is shown not to possess these pathological properties.

Some simple models with random hopping potentials are investigated in §5. For the linear chain, a slight disordering of the potentials localizes all the states with the consequent absence of a mobility edge, whilst in three dimensions it turns out that a mobility edge exists, and is likely to be found in the tail of the level density. Calculations based on a simple model suggest that it occurs when the density of states falls to 1/10 or 1/20 of the value at the band edge of the ordered crystal.

2. The Anderson model

The model introduced by Anderson (1958) consists of atoms situated at lattice sites interacting through nearest neighbours with a constant potential V . The disorder is introduced by stipulating that the energy levels associated with the sites are independent stochastic variables uniformly distributed over a range W .

Initially, we consider the one dimensional case, when the Hamiltonian is

$$H_{nm} = E_n \delta_{nm} + V \delta_{n,m \pm 1}. \quad (2.1)$$

The energy levels are given by the eigenvalues, say $\mathcal{E}_1^{(N)} \dots \mathcal{E}_N^{(N)}$ of equation (2.1), which are nondegenerate and all lie inside an interval of width $W + 4V$ (Varga 1962, p 16). The Green matrix associated with equation (2.1) is simply the matrix inverse of $(zI - H)$, where z is a complex energy value. The corner element in a 'site label' representation (or the off diagonal Green function) is given by

$$G_{1N} = \frac{\{\text{cofactor}(zI - H)\}_{1N}}{\det(zI - H)} = \frac{(-V)^{N-1}}{D_N} \quad (2.2)$$

where D_N is the determinant of $(zI - H)$.

Let us choose a particular energy eigenvalue, say $\mathcal{E}_\alpha^{(N)}$. Then the residue of the pole at $\mathcal{E}_\alpha^{(N)}$ in G_{1N} is

$$R_{1N}(\mathcal{E}_\alpha^{(N)}) = \frac{(-V)^{N-1}}{\prod_{k \neq \alpha} (\mathcal{E}_\alpha^{(N)} - \mathcal{E}_k^{(N)})}. \quad (2.3)$$

By definition, this residue is also given by

$$\langle 0 | a_1 | \alpha \rangle \langle \alpha | a_N^\dagger | 0 \rangle$$

where $|0\rangle$ refers to the electron vacuum and $|\alpha\rangle$ denotes an eigenstate. This residue is simply the product of the amplitudes of the wavefunction belonging to the state $\mathcal{E}_\alpha^{(N)}$ at the first and last sites; it also represents the probability amplitude for a particle in the eigenstate with energy $\mathcal{E}_\alpha^{(N)}$ to tunnel through the chain (cf Appendix). If the state is localized then we expect R_{1N} to decrease in an exponential manner as N increases.

We now assume that the energy eigenvalues $\mathcal{E}_k^{(N)}$ are distributed with the density of states $n(E)$, which for $W \gg 2V$ is approximately rectangular (Brouers 1970, private communication).

$$n(E) = \frac{1}{W} \quad -\frac{W}{2} < E < \frac{W}{2}. \quad (2.4)$$

We now express the residue $|R_{1N}(\mathcal{E}_\alpha^{(N)})|$ as $\exp(S_{N-1})$ where

$$S_{N-1} = (N - 1) \ln V - \sum_{j \neq \alpha} \ln |\mathcal{E}_\alpha^{(N)} - \mathcal{E}_j^{(N)}| \tag{2.5}$$

and assuming for the moment that the eigenvalues are independent of each other, we obtain for the probability density of $|R_{1N}|$

$$\left(\frac{2V}{W}\right)^{N-1} \frac{\left\{ (N - 1) \ln \frac{W}{2V} + \ln |R_{1N}| \right\}^{N-2}}{(N - 2)! |R_{1N}|^2} \tag{2.6}$$

for $(2V/W)^{N-1} < |R_{1N}| < \infty$.

The probability that $|R_{1N}(0)| < (1/y)^{N-1}$, for $y > 1$, is given by

$$1 - \exp \left\{ -(N - 1) \ln a \right\} \sum_{k=0}^{N-2} \frac{\{(N - 1) \ln a\}^k}{k!} \tag{2.7}$$

where $a = W/2Vy$. Provided $a > e$, the series in equation (2.7) increases monotonically and is therefore bounded by

$$\text{const} \times (N - 1)^{1/2} \times \left(\frac{e \ln a}{a}\right)^{N-2} \tag{2.8}$$

Hence equation (2.8) is exponentially small when

$$\frac{e \ln a}{a} < 1. \tag{2.9}$$

If $a < e$, the method of steepest descents demonstrates that equation (2.7) tends exponentially to zero. Hence the residue R_{1N} almost certainly tends to zero exponentially with the state localized, provided

$$\frac{W}{2V} > e. \tag{2.10}$$

This is the result that would be obtained by Anderson's method in one dimension.

The important feature of the distribution of the residue in equation (2.6) is its long tail. As Anderson and Thouless have emphasized in connection with the diagonal Green function, this means that the central limit theorem cannot be applied to the sum in $\ln |R_{1N}|$. However, since the residue is bounded by unity, this long tail is spurious and a proper treatment of the correlations between the eigenvalues must remove it. To lessen the effect of the tail, the distribution of $\ln |R_{1N}|$ is approximated by a Gaussian, and consequently

$$S_{N-1} = \ln |R_{1N}| = (N - 1) \left\{ \ln V - \int \ln |\mathcal{E}_\alpha^{(N)} - \mathcal{E}| n(\mathcal{E}) d\mathcal{E} \right\} + (N - 1)^{1/2} f \tag{2.11}$$

where the fluctuation term f has a Gaussian distribution. The condition for localization is now dependent on the negative nature of the mean in equation (2.11), and independent of the fluctuation term. At the centre of the band this gives the same condition as in equation (2.10). In one dimension, correlations between the eigenvalues do not affect the critical value of $W/2V$ but act in a way to cut off the distribution of the residue beyond unity.

The average in equation (2.11) can be evaluated for states away from the centre of the band and might lead to the possibility of mobility edges (Ziman 1969). For example, if the average is evaluated for the distribution (2.4) at the 'band edge' $\mathcal{E}_\alpha^{(N)} = W/2$, the condition for localization becomes

$$\frac{W}{V} > e. \tag{2.12}$$

However, it is unlikely that a mobility edge exists in the one dimensional case because the distribution (2.4) becomes inaccurate when W is of the order of $2V$ and thus equation (2.12) is not correct. When $W = 0$, the states are extended and the brace in equation (2.11) is zero. When W increases, the density of states is broadened and this tends to increase the integral in equation (2.11) favouring localization. Nevertheless, equation (2.12) indicates that it is easier for disorder to localize states lying near the band edge. This conclusion can also be reached from the intuitive approach given in the Appendix.

The same condition for localization can be obtained by investigating the residue R_{ij} between interior sites i and j . A complicating factor in this case is that equation (2.3) is multiplied by two determinants similar to D_N but of lower order. Here the off diagonal Green function is

$$G_{ij} = \frac{D(1 \dots i-1)(-V)^{j-i} D(j+1, \dots N)}{D(1 \dots N)}. \quad (2.13)$$

Where $D(1 \dots i-1)$ is the determinant for a chain with local site energies $E_1 \dots E_{i-1}$. When the determinants are diagonalized equation (2.13) becomes

$$G_{ij} = \frac{\prod_{k=1}^{i-1} (z - \mathcal{E}_k^{(i-1)}) \prod_{k'=j+1}^N (z - \mathcal{E}_k^{(N-j)}) (-V)^{j-i}}{\prod_{k'=1}^N (z - \mathcal{E}_k^{(N)})}. \quad (2.14)$$

When states are localized there is strong correlation between the energies $\mathcal{E}_q^{(i)}$ and $\mathcal{E}_q^{(N)}$ and the separation between the nearest levels tends exponentially to zero as $i \rightarrow N$. This is because, in the localized phase the perturbation caused by increasing the size of the system, has an exponentially small shifting effect on the initial spectrum. Thus the residue of the pole of equation (2.14) is a product like that in equation (2.3) but multiplied by a term

$$\prod_{k=1}^{i-1} \left(\frac{\mathcal{E}_\alpha^{(N)} - \mathcal{E}_k^{(i-1)}}{\mathcal{E}_\alpha^{(N)} - \mathcal{E}_k^{(N)}} \right) \prod_{k'=j+1}^N \left(\frac{\mathcal{E}_\alpha^{(N)} - \mathcal{E}_k^{(N-j)}}{\mathcal{E}_\alpha^{(N)} - \mathcal{E}_k^{(N)}} \right) \quad (2.15)$$

which is of the order of unity, when the states are localized.

We now consider the three dimensional lattice case. Feenberg (1948) has shown that the perturbation expansions for the residue of a pole at \mathcal{E}_0^M of the off diagonal Green matrix G_{ij} can be partially summed into a finite series of terms containing renormalized energy denominators. Thus if K is the connective constant for the lattice of M atoms (Anderson 1958), then

$$R_{ij}(\mathcal{E}_0^M) = \sum_{N > |i-j|}^M \sum_{K_{\text{paths}}^N} \prod \frac{(-V)}{(\mathcal{E}_0^M - \mathcal{E}_k^{(N)})}. \quad (2.16)$$

The summation is over distinguishable nonrepeating paths connecting sites i and j . The renormalized levels are $\mathcal{E}_k^{(N)}$, also discussed by Anderson, which depend not only on \mathcal{E}_0^M but on the path on which $\mathcal{E}_k^{(N)}$ lies.

For the localized phase, we have already seen that increasing the size of the system has little effect on the energy levels. This must also be true for the renormalized local levels and consequently we approximate these levels by the exact eigenvalues. This replacement is consistent with the analytical properties of the Green function and reduces to the exact results in the one dimensional case. Because it neglects the dependence of $\mathcal{E}_k^{(N)}$ on \mathcal{E}_0^M , we call it the static approximation. Effectively Anderson and Thouless make the same assumption for the case $W \gg 2V$.

The renormalized local levels $\mathcal{E}_k^{(N)}$ are not statistically independent and two distinct types of correlation are distinguished: (i) correlation between sets of levels belonging to distinct paths, (ii) correlation between levels on the same path.

When the first type of correlation is neglected, it follows from the fact that the residue R_{ij} is bounded by unity, that the variance of each product in equation (2.16) must be finite. Correlation of the second type must therefore be active in eliminating tails in the distribution of the products in equation (2.16). When this is also neglected, Anderson's upper estimate of the critical value of $W/2V$ is obtained. Lower estimates are then derived by including correlation of the second type, using the Gaussian assumption already discussed for the one dimensional case, and also by introducing a cut off at K^{-N} for the distribution of the product. However, correlation of the first type and corrections to the static approximation can allow the values of the products in equation (2.16) to exceed K^{-N} . The static approximation is expected to be good in the localized region, and in this case contributions from the tail of the distribution of the product would be removed by cancellation in the summation in equation (2.16). It is argued that even in this case an upper bound for the cut off of f would be of order \sqrt{N} , and consequently the Gaussian distribution for f should lead to an upper estimate for the value of the residue. A lower estimate for the critical value of $W/2V$ is obtained by choosing the path which gives the maximum contribution to equation (2.16). This path is defined by a chain of neighbouring sites having renormalized local levels lying closest to the energy eigenvalues $\epsilon_0^{(M)}$. It is encouraging to note that these estimates obtained by including correlations are not widely different.

2.1. Neglect of all types of correlation

In this case the distribution of each product in equation (2.16) is given by equation (2.6). This has the form, if $|R_{ij}| = X$

$$P(X \leq x) = 1 - \frac{L(x)}{x} \tag{2.17}$$

for $x > (2V/W)^N$, where $L(x)$ is a slowly varying function at $x = \infty$. The distribution of a sum of K^N independent variables each with a distribution of this form is asymptotically

$$1 - \frac{K^N L(x)}{x}$$

(Feller 1966, p. 271), since the distribution of the sum is dominated by the largest term.

The probability that this sum is greater than $(1/y)^N$ is less than

$$\text{const} \times \left\{ \frac{eK \ln(W/2Vy)}{W/2Vy} \right\}^N \tag{2.18}$$

provided $W/2Vy > e$. The condition that equation (2.18) tends to zero for all $y > 1$, is

$$\frac{W}{2V} > eK \ln \frac{W}{2V}. \tag{2.19}$$

This condition is the same as Anderson's upper limit.

2.2. Partial account of type-two correlations

The form of the product in equation (2.16) is the same in three as in one dimension. We know that in the latter case, correlations between levels must act to reduce the long tail of the distribution of the product so that its variance is finite.

We propose to estimate this variance by approximating the distribution of S_N by equation (2.11). Let us suppose the mean and variance of S_N are Nm and $N\sigma^2$ respectively. Then the sum of $\exp(S_N)$ over independent distinct paths in equation (2.16) is dominated by

$$X = \sum_{KN} \exp(S_N). \tag{2.20}$$

The mean $\langle X \rangle$, and variance, $\text{var } X$, of X are, respectively, just

$$\{K \exp(m + \sigma^2/2)\}^N \quad \text{and} \quad \{K \exp(2m + 2\sigma^2)\}^N.$$

Now Chebycheff's inequality (Feller 1966) implies that

$$P(|X - \langle X \rangle| \geq t) \leq \frac{\text{var } X}{t^2}$$

for all values of $t > 0$.

Hence provided $\text{var } X < \langle X \rangle^2$, that is

$$\ln K > \sigma^2 \quad (2.21)$$

X is dominated by its mean value which tends to zero exponentially when

$$m + \frac{\sigma^2}{2} + \ln K < 0. \quad (2.22)$$

Consequently the residue tends to zero exponentially when equations (2.21) and (2.22) are satisfied. For the density of states given in equation (2.4), at the centre of the band $m = \ln(W/2V) - 1$, $\sigma^2 = 1$.

Hence for $K > e$, the condition for localization is

$$\frac{W}{2V} > e^{3/2} K. \quad (2.23)$$

This is considerably weaker than Anderson's upper limit and best estimate.

2.3. Alternative treatment of type-two correlations

A second approach to the distribution of S_N given by equation (2.11) is to cut off the fluctuation term f so that

$$\exp(S_N) < K^{-N}.$$

This simply means that fluctuations can never delocalize the states, and the condition for localization at the centre of the band is given by equation (2.22) with $\sigma^2 = 0$

$$\frac{W}{2V} > Ke. \quad (2.24)$$

This estimate was also derived by Ziman using a rather different approach. Equation (2.24) can also be obtained directly from the distribution in equation (2.6) by introducing a cut off at K^{-N} . Hence when correlations of type two are fully accounted for by forcing the residue to be less than unity, the condition for localization (2.24) does not depend on the central limit theorem.

2.4. A lower limit to the critical value of $W/2V$

To derive a lower limit to the localization region, we select out of equation (2.16) the path which gives the maximum contribution. This occurs when the energy denominators are as small as possible. If the renormalized local levels have the distribution given in equation (2.4), then for $\mathcal{E}_0^{(M)}$ lying at the centre of the band, the probability density for the renormalized energy level \mathcal{E} of a nearest neighbour site having \mathcal{E} closest to the eigenvalue (with the exception of the previous member of the path) is

$$f(\mathcal{E}) = \frac{(z-1)}{a} \left(1 - \frac{\mathcal{E}}{a}\right)^{z-2} \quad (2.25)$$

where a is $W/2$ and z is the coordination number. The average value of S_N in equation (2.11) is then

$$N \left[\ln \frac{V}{a} - (z-1) \left\{ -1 + \left(\frac{z-2}{4} \right) - \frac{(z-2)(z-3)}{9 \cdot 2!} + \dots \right\} \right]. \quad (2.26)$$

The fluctuations for this expression can be neglected because they are of the order \sqrt{N} . Consequently the electron will be unable to tunnel if, for $z = 6$

$$\frac{W}{2V} > e^{2.3}. \quad (2.27)$$

This represents a lower limit because the electron may be propagated through a large number of paths whereas we have only considered one. However, when the spread of local levels becomes large, the wavefunctions will concentrate along paths of this type and hence correlations may force the condition for localization close to (2.27). This estimate is similar to one devised by Thouless (1970, equation (19)).

The expression (2.26) gives the maximum value of S_N and consequently it can be used to obtain an upper estimate for the cut off on the distribution for f . By comparing equation (2.26) with equation (2.11) it can easily be shown that $f < \alpha\sqrt{N}$, where α is of order one. Consequently the Gaussian approximation in equation (2.11) is expected to give a good upper estimate of the condition for localization.

The conditions for localization have been obtained at the centre of the band. However, away from the centre, the relevant integrals can still be evaluated and the condition for localization becomes energy dependent, thus leading to the concept of a mobility edge (cf Ziman 1969).

3. Wavefunctions for the linear chain

We have seen in §2 that the eigenvalues of the N atom chain are denoted by $x_1^{(N)} \dots x_v^{(N)} \dots$ and satisfy

$$D_N = 0. \quad (3.1)$$

The determinant of the $p \times p$ matrix whose elements are

$$(x - E_k) \delta_{k,l} - V \delta_{k,l \pm 1} \quad (3.2)$$

is denoted by D_p and satisfies the recurrence relation

$$D_p - (x - E_p) D_{p-1} + V^2 D_{p-2} = 0 \quad (3.3)$$

with initial conditions $D_0 = 1$, $D_1 = (x - E_1)$. For convenience, in this and the following section we choose a unit of energy such that $V = 1$. Then equation (3.3) reduces to the definition of the unnormalized eigenvectors with $x = x_v^{(N)}$. It is possible to deduce information about the asymptotic behaviour of $D_n(x)$ in two cases. The first case corresponds to the situation where the amplitudes D_n and the local levels vary slowly with n , and occurs when there is intensive correlation between the levels. The second case corresponds to the Anderson model, where E_n are independently distributed.

In the first case, the WKB method demonstrates that $D_n(x)$, and hence the wavefunction, oscillate sinusoidally with slowly varying amplitude for values of n satisfying $|(E_n - x)/2V| < 1$. Otherwise $D_n(x)$ behaves like an exponential function of n (Dingle and Morgan 1967). A disordered system in which the local levels were correlated in this manner would then behave like a sequence of metal-insulator junctions and the variance of the wavefunction could be infinite. We expect that similar behaviour may occur on the delocalized side of the transition, where the density of states must adjust itself to the local levels so that the term in the exponent of R_{ij} is never positive, otherwise R_{ij} would not be bounded by unity. Consequently over a large number of sites R_{ij} will change slowly and each wavefunction amplitude must then be of order $1/\sqrt{N}$. It is this readjustment of the density of states to the local levels which makes it so difficult to discuss the transition region in detail.

In the second extreme case, the local levels are independent of each other. The amplitudes have the form

$$D_n = \prod_{i=1}^N (x - x_i^{(N)})$$

where $x_i^{(N)}$ are the eigenvalues of the n level system. From the analysis of the off diagonal propagator in §2 it follows that if the condition for localization (2.22) is satisfied, D_n tends to increase exponentially. It is convenient to consider the probability density $f_n(x)$ of the quotient $\omega_n = D_n/D_{n-1}$ for values of energy in the centre of the band. Then if $W/2 > |\omega|$, $V = 1$

$$f_n(\omega) = \frac{1}{W} \left\{ 1 - \int_{\frac{-1}{W/2 + \omega}}^{\frac{1}{W/2 - \omega}} f_{n-1}(\omega') d\omega' \right\}. \tag{3.4}$$

This equation can be approximately solved, for $W/2 \gg |\omega|$, by integrating the left hand side from $-\{(W/2) + \omega\}^{-1}$ to $\{(W/2) - \omega\}^{-1}$. The solution is then

$$f_n(\omega) = \frac{1}{W} \left\{ 1 - \frac{1}{(W/2)^2 + \omega^2} \right\} \tag{3.5}$$

and when $|\omega| \gg W/2$, f_n can be shown to decrease like $1/W\omega^2$.

From this, two important conclusions can be drawn. Firstly, $f_n(\omega)$ quickly becomes independent of n , and secondly the probability that $|\omega| < 1$ is quite small ($\simeq 2/W$); consequently $|D_n(0)|$ is likely to be greater than $|D_{n-1}(0)|$. If we start to solve the recurrence relation (3.3) from the other end of the chain, we are likely to find that the solution also increases from that end. It is therefore necessary to explain how $D_n(x_v^{(N)})$ can turn over at some point in the chain and then decrease (on average) until the end of the chain, where $D_N(x_v^{(N)}) = 0$. We have shown in §2 that the residue of a pole in G_{1N} almost certainly decreases in an exponential manner. This is only true if the shift of the roots caused by increasing N is small. To calculate the shift, we assume that $D_k(x)$ is given by

$$D_k(x) = D'_k(x_k)(x - x_k) \tag{3.6}$$

for x in the neighbourhood of a root x_k of $D_k(x)$.

From the recurrence relation (3.3) we deduce that

$$\frac{x_{k+1} - x_k}{x_k - x_{k-1}} = \frac{D'_{k-1}(x_k)}{D'_{k+1}(x_{k+1})}. \tag{3.7}$$

Now if $|D'_k(x_k)|$ increases at a rate γ so that

$$|D'_k(x_k)| \simeq \exp(\gamma k) |D'_1(x_1)| \tag{3.8}$$

then $|x_{k+1} - x_k|$ decreases at a rate 2γ so that

$$|x_{k+1} - x_k| \simeq \exp(-2\gamma k) |x_2 - x_1|. \tag{3.9}$$

Consequently we expect that $D_n(x_v^{(N)})$ increases on average until a local level E_{m_0} is introduced, which produces a root of D_m lying close to $x_v^{(N)}$ such that equation (3.6) is valid. Then for $m > m_0$

$$\begin{aligned} |D_m(x_v^{(N)})| &\simeq |D'_m(x_m)| |(x_v^{(N)} - x_v^{(N-1)}) + \dots (x_{m+1} - x_m)| \\ &\sim \exp(m\gamma) [\exp(-2N\gamma) + \exp\{-2(N-1)\gamma\} + \dots \exp(-2m\gamma)] |D'_1(x_1)| \\ &\sim \exp(-m\gamma) |D'_1(x_1)|. \end{aligned} \tag{3.10}$$

Hence, although $|D_m(x)|$ continues to increase, $|D_m(x_v^{(N)})|$ decreases on average for $m > m_0$. This explains the turnover and shows that the centre of the localized wavefunction is likely to be at the position of the local level which lies closest to the eigenvalue.

However, the behaviour of $|D_n(x_N)|$ is not smooth, as there will be fluctuations about the exponential. The presence of a second level x_m close to x_N means that $|D_m(x_N)| \simeq |D_{m-2}(x_N)|$ and $|x_m - x_{m-1}| \simeq |x_{m-1} - x_{m-2}|$. Nevertheless, the variance of these wavefunctions is almost certainly finite, even though their centres are independent random variables, and hence the static conductivity is almost certainly zero (Halperin 1968).

4. The selfenergy for a linear chain

Considerable confusion has been caused by the strange analytical behaviour of the selfenergy associated with the Green matrix (Anderson 1970). We now consider in detail the analytical properties of the selfenergy in the different regions and also the effect of averaging the selfenergy or Green matrix. For convenience we choose $V = 1$, although the analysis is also applicable to the case of variable V , provided each V is of definite sign. The diagonal elements of the Green matrix are given by

$$\frac{\{\text{cofactor}(zI - H)\}_{ii}}{\det(zI - H)}$$

which can be expanded into the form

$$\{z - E_i - (\Sigma_1 + \Sigma_2)\}^{-1}. \tag{4.1}$$

We denote the determinant of $(zI - H)$ for a system with i atoms whose local levels are E_1, \dots, E_i by $D(1 \dots i)$. Then

$$\Sigma_1 = \frac{D(1 \dots i - 2)}{D(1 \dots i - 1)} \tag{4.2}$$

$$\Sigma_2 = \frac{D(i + 2, \dots N)}{D(i + 1, \dots N)}. \tag{4.3}$$

The selfenergy is just $\Sigma_1 + \Sigma_2$. Since the levels are independent, we may consider without loss of generality only the quantity Σ_2 , for the case $i = 0$. We can then denote $D(1 \dots N)$ by D_N and $D(2 \dots N)$ by Q_N . The zeros of D_N and Q_N correspond to the eigenvalues of the $(N - 1)$ and $(N - 2)$ level systems respectively, and consequently the selfenergy has poles at the eigenvalues of the $(N - 1)$ level system and zeros at the eigenvalues of the $(N - 2)$ level system. It is evident that the selfenergy of G_{00} is simply G_{11} and can be written in the form

$$\Sigma_{00}(x) = \sum_x \frac{\langle 1|\alpha\rangle \langle \alpha|1\rangle}{(x - \mathcal{E}_\alpha)}$$

where \mathcal{E}_α is the eigenvalue of the $(N - 1)$ level system, and $|\alpha\rangle$ denotes the corresponding eigenstate. $|1\rangle$ is the Wannier state $a_1^\dagger|0\rangle$. If the eigenstates are localized, the residues at the poles of Σ_{00} form an exponentially decreasing series with the sum rule $\sum_x \langle 1|\alpha\rangle \langle \alpha|1\rangle = 1$. This sum rule can be satisfied to any required degree of accuracy by a finite number of residues, so that the selfenergy has a discrete pole structure, and in the limit as the length of the chain tends to infinity, the imaginary part of the selfenergy is zero, except at a discrete set of points. We now consider this situation in more detail.

It is clear that D_N and Q_N satisfy the recurrence relation

$$D_N = (x - E_N) D_{N-1} - D_{N-2} \tag{4.4}$$

with initial conditions

$$\left. \begin{aligned} D_0 &= 1 & D_1 &= (x - E_1) \\ Q_0 &= 0 & Q_1 &= 1. \end{aligned} \right\} \tag{4.5}$$

Consequently D_n and Q_{n+1} are orthogonal polynomials of the first and second kind, of degree n in x , since there exists a weight function $\sigma(x)$ such that

$$\int D_n(x) D_m(x) \sigma'(x) dx = \delta_{nm}. \tag{4.6}$$

If we denote the zeros of $D_N(x)$, which give the energy values, by $x_v^{(N)}$, then, as we have already

seen in §3, the normalized amplitude of the wavefunction on site k is just

$$\frac{D_{k-1}(x_v^{(N)})}{\left\{ \sum_1^N D_{k-1}^2(x_v^{(N)}) \right\}^{1/2}} \tag{4.7}$$

A considerable number of properties of these orthogonal polynomials are known (cf Szegő 1939, Shohat and Tamarkin 1943, Akhiezer 1965). For example: (i) the zeros of D_n and Q_n are all real and simple; (ii) any two zeros of D_n are separated by a zero of D_{n-1} and vice versa; (iii) any two zeros of Q_n are separated by a zero of D_n and vice versa; (iv) the Darboux-Christoffel formula tells us that

$$\sum_0^{n-1} D_k^2(x) = D_{n-1}(x) D'_n(x) - D_n(x) D'_{n-1}(x)$$

(v) the Liouville equation gives

$$D_{n-1}(x) Q_n(x) - D_n(x) Q_{n-1}(x) = 1.$$

From these properties it is clear that $\Sigma_2(x)$ is a function with N poles at $x_v^{(N)}$ (that is, the eigenvalues of the system which has one atom less) and $N - 1$ zeros at $x_v^{(N-1)}$. We know from property (iii) that these points are all distinct but become closer as the size of the system increases, and it is remarkable that any perturbation series for $\Sigma_2(x)$ can converge at all!

We now make a partial fraction expansion of $\Sigma_2(x)$:

$$\Sigma_2(x) = \sum_{v=1}^N \frac{R_N(x_v^{(N)})}{x - x_v^{(N)}} \tag{4.9}$$

where the residue has the form

$$R_N(x_v^{(N)}) = \frac{Q_N(x_v^{(N)})}{D'_N(x_v^{(N)})}.$$

From properties (iv) and (v), this is simply

$$\left\{ \sum_0^N D_k^2(x_v^{(N)}) \right\}^{-1} \tag{4.10}$$

which is simply related to the normalization constant for the wavefunctions in equation (4.7), and its value indicates the nature of the states. The residue obeys the sum rule

$$\sum_{v=1}^N R_N(x_v^{(N)}) = 1. \tag{4.11}$$

To see this, we note that the selfenergy $\Sigma_2(x)$ is the N th approximant to a continued fraction (Wall 1965):

$$\frac{1}{x - E_N - \frac{1}{x - E_{N-1} - \frac{1}{\dots - \frac{1}{x - E_1}}}} \tag{4.12}$$

Clearly the fraction (4.12) can be expanded in an asymptotic series

$$\frac{Q_N(x)}{D_N(x)} = \Sigma_2(x) = \sum_{k=0}^{\infty} \frac{\mu_k}{x^{k+1}} \tag{4.13}$$

where μ_k are constants, and $\mu_0 = 1$; comparing equation (4.13) with the expansion (4.9), we deduce that

$$\sum_{v=1}^N (x_v^{(N)})^k R_N(x_v^{(N)}) = \mu_k. \tag{4.14}$$

Putting $k = 0$ in equation (4.14) we obtain equation (4.11).

As an example let us consider a periodic system where all the E_n are equal to E_0 . The difference relations (4.5) imply that in this case

$$\Sigma_2(x) = \frac{\sinh(N \ln Z)}{\sinh\{(N + 1) \ln Z\}} \tag{4.15}$$

where

$$Z = \left(\frac{x - E_0}{2}\right) + \left\{\left(\frac{x - E_0}{2}\right)^2 - 1\right\}^{1/2}. \tag{4.16}$$

$D_n(x)$ is equal to zero only when $|(x - E_0)/2| < 1$. If we write $(x - E_0)/2 = \cos \theta$, it is clear that $D_n(x)$ and $Q_n(x)$ are closely related to the Chebycheff polynomials of the first and second kinds (Szegö 1939). If x lies in the band

$$\Sigma_2(x) = \frac{\sin N\theta}{\sin(N + 1)\theta}. \tag{4.17}$$

Clearly no perturbation series for equation (4.17) can converge when N tends to infinity. For x outside the band Σ_2 converges to

$$\frac{\text{sign}(x - E_0)}{|(x - E_0)/2| + [\{(x - E_0)/2\}^2 - 1]^{1/2}} \tag{4.18}$$

and we can expand this quantity in an asymptotic series like (4.13). It can be shown that this series is the same as that obtained by expanding the integral

$$\frac{2}{\pi} \int_{-1}^{+1} \frac{(1 - u^2)^{1/2} du}{\{(x - E_0)/2 - u\}} \tag{4.19}$$

and that the above representation is unique.

The interpretation of equation (4.17) is that the separation of the poles of the partial fraction (4.9) is $O(1/N)$. The residue, from the term of (4.10), is $O(1/N)$. Hence the expression (4.9) converges to the Riemann integral (4.19) which is analytical everywhere when x is not in the band. For x in the band, however, the expression (4.19) defines a function with a cut along the real axis. The discontinuity across this cut is the imaginary part of $(1/\pi)\Sigma_2(x)$, which, by an inversion formula (Wall 1965), is just

$$\frac{2}{\pi} \left\{1 - \left(\frac{x - E_0}{2}\right)^2\right\}^{1/2}.$$

This is the imaginary part of the selfenergy, which is connected with the decay time of the time dependent propagator. Its existence here is due to the fact that the Wannier site representation which we have been using does not diagonalize the Hamiltonian.

In general the expression (4.9) can be written in the form of an integral:

$$\Sigma_2(x) = \int_a^b \frac{\sigma'(u) du}{x - u}. \tag{4.20}$$

Here a and b are the extremes of the band, and

$$\sigma'(u) = \lim_{N \rightarrow \infty} \sum_{v=1}^N \delta(u - x_v^{(N)}) R_N(x_v^{(N)}) \tag{4.21}$$

where $\sigma(u)$ is the weight or distribution function. Equation (4.14) now reduces to

$$\int_a^b u^k \sigma'(u) du = \mu_k. \tag{4.22}$$

The determination of the function $\sigma(u)$ from the moments μ_k is known as the moment problem for a finite interval. The conclusions of studies of this problem (Akhiezer 1965, Shohat and Tamarkin 1943) assure us that if the potentials V_n are of definite sign such that $\sum_1^\infty 1/|V_n|$ is divergent, then the moment problem has an essentially unique solution. The solution $\sigma_N(u)$ for a system of size N is nondecreasing, and continuous everywhere except at the points $x_v^{(N)}$, where the discontinuity is

$$\sigma_N(x_v^{(N)+}) - \sigma_N(x_v^{(N)-}) = R_N(x_v^{(N)}). \tag{4.23}$$

The generalization of the inversion formula (Akhiezer 1965), for any interval (c, d) is

$$\lim_{\epsilon \rightarrow 0} \frac{1}{\pi} \int_c^d \text{Im} \Sigma_2(x + i\epsilon) dx = \sigma(d) - \sigma(c). \tag{4.24}$$

We are now able to consider the selfenergy on both sides of the transition region.

On the delocalized side, from §3, we expect that $\sum_m^{N+m} D_n^2(x_v) = O(N)$, for some value of m . Consequently we expect $\sigma(u)$ to be a continuous function in this case except possibly at a number of isolated points. The imaginary part of the selfenergy would not then be always zero. On the localized side, we expect $D_n(x_v^{(N)})$ to tend to decrease on average as $|n - v|$ increases (§ 3), so that the residue $R_n(x_v^{(N)})$ tends to behave like an exponentially decreasing series in v . The distribution function $\sigma'(x)$ in equation (4.21) does not converge in any sense. In any finite interval of the band, the imaginary part of $\Sigma_2(x)$ is concentrated on a discrete set of points and is zero in between. (This agrees with the remarks of Anderson 1970 and Thouless 1970.)

These properties disappear on averaging. For example, consider the corner element of the Green matrix $G_{11}(x + i\epsilon)$. This has the (convergent) continued fraction expansion (4.12) with x replaced by $x + i\epsilon$. We assume that the local levels have a Cauchy distribution

$$P(E) = \frac{\alpha}{\pi(E^2 + \alpha^2)} \tag{4.25}$$

and make use of the identity

$$\int_{-\infty}^{+\infty} f(E) P(E) dE = f(-i\alpha) \tag{4.26}$$

provided that $f(E) = O(1)$ as $E \rightarrow \infty$, and $f(E)$ has no poles in lower half plane. We now apply the identity (4.26) to $f(E_1) = G_{11}(x + i\epsilon, E_1, E_2 \dots E_N)$, noting that both the required conditions are satisfied (Wall 1965, p 72, proves that $G_{11}(x + i\epsilon)$ has no poles in the lower half plane when $E_1 \dots E_N$ lie there) and obtain

$$\begin{aligned} \langle G_{11}(x + i\epsilon) \rangle &= \langle \Sigma_2(x + i\epsilon) \rangle \\ &= \int \frac{(1 - u^2)^{1/2} du}{\{(x + i\alpha)/2 - u\}}. \end{aligned} \tag{4.27}$$

The averaged selfenergy or Green function can be seen to possess an imaginary part (cf Lloyd 1969). Thus the averaging destroys the discrete pole structure and the imaginary part of $\langle \Sigma_2 \rangle$ cannot be interpreted as an inverse lifetime. Also an essential difficulty with the Cauchy distribution seems to be that it is too broad, so that no moments can be defined.

5. Randomized hopping potentials

The local levels are now assumed to be equal and the hopping potentials V_n random

variables. We need to examine the distribution of the product

$$\prod_{j=1}^N \frac{V_j}{|E - \mathcal{E}_j|} \quad (5.1)$$

where \mathcal{E}_j are the renormalized 'local' levels whose distribution we shall take to be given by the density of states. In our model, we consider the potentials to be independently distributed with a uniform density

$$1 - \epsilon < V_j < 1 + \epsilon. \quad (5.2)$$

In one dimension the residue can be written in the form

$$\exp \{N \langle \ln V - \ln |\mathcal{E}| \rangle + f \sqrt{N}\}.$$

The fluctuation term f is negligible and for the periodic case, $\langle \ln V \rangle$ and $\langle \ln |\mathcal{E}| \rangle = 0$. As the system is disordered ($\epsilon > 0$), $\langle \ln V \rangle$ decreases and $\langle \ln |\mathcal{E}| \rangle$ tends to increase. Thus we expect all states to be localized in the one dimensional case. It is interesting to consider this case in more detail. For the linear chain, the density of states is given by its average periodic value for energies not too far from the centre of the band:

$$n(E) = \frac{1}{\pi(4 - E^2)^{1/2}}. \quad (5.3)$$

It is clear that a necessary condition for localization is

$$\text{Prob} \left(\frac{V}{|E - \mathcal{E}|} > 1 \right) < \frac{1}{2}. \quad (5.4)$$

We thus expect conditions for localization to be more favourable at the band edges. At the centre of the band, $E = 0$, and the condition (5.4) is true for $\epsilon > 0$. Since condition (5.4) is insufficient to prove localization, we require the probability density of $y = V/|x - \mathcal{E}|$, which for large y is given by

$$f(y) = \frac{1}{2\epsilon} \int_{\frac{1-\epsilon}{y}}^{\frac{1+\epsilon}{y}} \eta \, d\eta \{n(E - \eta) + n(E + \eta)\}. \quad (5.5)$$

For $\epsilon = 1$, and $E = 0$

$$f(y) = \begin{cases} \frac{2}{\pi} & 0 < y < 1 \\ \frac{2}{\pi} \left\{ 1 - \left(1 - \frac{1}{y^2} \right)^{1/2} \right\} & y > 1 \end{cases} \quad (5.6)$$

It is difficult to evaluate the distribution of $\prod_{j=1}^N y_j$, by the technique given in § 2, owing to the Fourier inversion. Hence we approximate the distribution of (5.1) by first of all concentrating on the tails of the distribution in (5.6),

$$f(y) = \begin{cases} \frac{2}{\pi} & 0 < y < 1 \\ \frac{1}{\pi y^2} & y > 1 \text{ say} \end{cases} \quad (5.7)$$

The probability that $y > 1$ is just $1/\pi$. Consequently in the sum $\sum_{j=1}^N \ln y_j$ we expect roughly N/π values of y_j such that $y_j > 1$ and the remainder having values less than 1.

The latter sum has a mean value of

$$N \left(1 - \frac{1}{\pi} \right) \frac{\int_0^1 \ln y f(y) dy}{\int_0^1 f(y) dy} \quad (5.8)$$

with fluctuations which are of order \sqrt{N} . The first part of the sum can be analysed by the techniques in §2. The result confirms our expectation that almost all the states in the band are localized. It is interesting to note that we can actually find a state which is not localized when $\epsilon \neq 1$. This occurs precisely at $E = 0$, and the recurrence relation for the eigenvector e_n becomes

$$V_n e_n + V_{n+1} e_{n+1} = 0 \quad (5.9)$$

with initial conditions $e_1 = 1$ and $e_2 = 0$. When N is even, $E = 0$ is an eigenvalue, and the corresponding eigenvector is

$$e_n = \begin{cases} (-1)^{(n-1)/2} \frac{V_1}{V_n} & n \text{ odd} \\ 0 & n \text{ even} \end{cases} \quad (5.10)$$

which is certainly not localized. Statistical arguments, however, show that the states around $E = 0$, are almost certainly localized (cf. Borland 1963).

The same conclusion is also reached when the distribution of $\ln V/|x - \mathcal{E}|$ is approximated by a Gaussian. We have already learnt that the fluctuations about the mean of $\ln V/|x - \mathcal{E}|$ are not important, and the mean is simply

$$\frac{(1 + \epsilon) \ln(1 + \epsilon) - (1 - \epsilon) \ln(1 - \epsilon) - 2\epsilon}{2\epsilon} \quad (5.11)$$

This is negative for $\epsilon > 0$ and hence localization is favoured. For $\epsilon = 0$, it is interesting to note that the mean actually becomes zero, confirming that the method is valid right up to the delocalization point in one dimension.

In three dimensions, we use the approximate density of states for the periodic crystal when $\epsilon = 0$:

$$n(E) = \frac{1}{18\pi} (36 - E^2)^{1/2} \quad (5.12)$$

Using this density, the residue at the centre of the band for the periodic case from equation (2.16) turns out to diverge like $\{K \exp(-0.6)\}^N$. This is inconsistent with the nature of the residue in a periodic assembly and may be due either to the density of states (5.12) being too crude for the tight binding cubic lattice, or to the static approximation becoming unjustified in the delocalized region. It would be interesting to use a more accurate density of states to compute the average for the periodic case.

To approximate the density of states for a disordered system we replace equation (5.12) by the density calculated by averaging the periodic density $(36V^2 - E^2)^{1/2}/18\pi V^2$, for $|E| < 6V$, over V given in equation (5.2). This has the effect of removing the Van Hove singularities and increasing the band width to $12(1 + \epsilon)$, and it gives a reasonable spectrum when ϵ is not too large. For $\epsilon = \frac{1}{2}$ it turns out that

$$m = \left\langle \ln \frac{V}{|E - \mathcal{E}|} \right\rangle = -1.46 \quad \text{for } E = 6$$

and

$$m = -2.12 \quad \text{for } E = 9$$

whereas $\sigma^2 = \text{var } V/|E - \mathcal{E}|$ is 1.33 for $E = 6$, and 0.8 for $E = 9$. This means that the upper limit associated with equations (2.21) and (2.22) is satisfied in the tail only when

$4.0 < K < 5.5$. In particular, if $K = 4.5$ (the value for a simple cubic lattice) a mobility edge lies in the tail. It is interesting that this edge occurs when the density of states has decreased by an order of magnitude from the level density at the band edge. As the density (5.12) gives a divergence for the residue in the periodic case, it is weighted towards delocalization in our approximations and consequently the existence of localized states in this calculation is strong evidence for a mobility edge in the tail.

6. Conclusion

It has been shown, within the limits of certain approximations, that the correlations between renormalized local levels, which have been neglected by previous authors, can have a considerable effect on the conditions for localization. Use of the off diagonal propagator greatly facilitates the analysis, and has led to new insight into the nature of the Anderson transition in disordered systems. For convenience, our results on cellular disorder are given in table 1.

Table 1. The conditions for localization at the centre of the band with cellular disorder; $W/2V > x$, $K = 4.5$.

Approximation	x
1. (a) Anderson's upper limit	45
(b) Anderson's best estimate	30
2. Gaussian approximation for the fluctuations	20
3. Neglecting the fluctuations	12
4. Percolation approximation	10

The Gaussian approximation for f is expected to give an upper estimate for the true value of the residue in the localized phase, and under the assumption that correlation between paths is not important, the approximation of neglecting fluctuations f gives an upper estimate for x consistent with the fact that the residue is bounded by unity. The percolation approach indicates that correlations may also reduce the effective connectivity constant. It is gratifying to note that the three estimates for x obtained by including correlation are quite close, and it is probable that the true value of x lies in the range 10–20 for a flat density of states. A more realistic density of states function would have a tail tending to increase the value of $\langle \ln |\mathcal{E}| \rangle$ thus favouring localization, and the above approach should therefore lead to upper estimates of x .

The treatment of disorder involving random hopping potentials is much more difficult, owing to the uncertainties in the static approximation for the renormalization and the sensitivity of effects to the form of the density of states. However, calculations indicate that all states are localized in one dimension, and in three dimensions there is probably a mobility edge in the tail of the distribution. In §3 we have attempted to present a detailed analysis of the analytic structure of the selfenergy which resolves the recent controversy raised by the work of Lloyd and gives a physical picture of the discrete pole structure in the localized phase.

All the work in this paper has concentrated on the one electron approximation, and it may be that interactions also have an important effect in producing localized states. To see how the electron–electron interaction could produce effective cellular disorder, it is instructive to consider the Hubbard Hamiltonian for correlation in narrow energy bands (Hubbard 1963). This can be written in the form

$$H = \sum_{i,\sigma} (E_0 + In_{i,-\sigma}) a_{i\sigma}^+ a_{i\sigma} + V \sum_{i,\delta,\sigma} a_{i\sigma}^+ a_{\delta\sigma}$$

The electron occupation number on any given site fluctuates in time due to band motion, and this has the effect of disordering the one electron local levels. A similar effect may occur in the disordered systems considered in this work. The ideas of the Anderson transition may also be relevant to the many body problem.

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Appendix. The physical mechanism of localization

In this section we give an intuitive interpretation of the structure of the residue of the off diagonal propagator, which gives some insight into the mechanism of localization. If the Hamiltonian is written in the form

$$H = \sum_i E_i a_i^+ a_i + \sum_{i,\delta} v_{i\delta} a_i^+ a_\delta$$

then by considering the time derivative of the number operator we are led to define a local velocity $\tilde{v}_{i\delta}$ by

$$\tilde{v}_{i\delta} = cv_{i\delta} \frac{\langle \alpha | a_i^+ a_\delta | \alpha \rangle}{\langle \alpha | a_i^+ a_i | \alpha \rangle}$$

where $|\alpha\rangle$ is an eigenstate and c is a constant depending on the lattice. This can also be written in the form

$$\tilde{v}_{i\delta} = cv_{i\delta} \frac{\alpha_\delta}{\alpha_i}$$

where $\alpha_\delta = \langle \alpha | a_\delta^+ | 0 \rangle$. If we consider the electron in an eigenstate tunnelling through the lattice then $\tilde{v}_{i\delta}$ has to be sufficient to broaden the renormalized local energy level to encompass the eigenvalue of the state $|\alpha\rangle$, and this gives a minimum value to the ratio α_δ/α_i . The broadening is given by the uncertainty principle

$$\begin{aligned} \Delta E \Delta t &\sim \hbar \\ \Delta E &\sim \frac{\hbar}{\Delta t} \sim \frac{\hbar v_i}{a} \end{aligned}$$

where a is the interatomic distance and hence

$$\tilde{v}_i \sim \frac{a}{\hbar} \Delta E.$$

If the electron tunnels from site 1 to site N , then the ratio of the wave function at these sites is

$$\frac{\alpha_N}{\alpha_1} \simeq \prod_i \frac{\Delta E_i}{v_{i\delta}}$$

where $\Delta E_i = (E_\alpha - E_i)$. This is the inverse of the residue in one dimension, and of the residue obtained in the percolation limit in three dimensions. If the residue tends to zero exponentially the wavefunction should be exponentially localized. Hence the factors $v_{i\delta}/\Delta E_i$ occurring in the residue can be interpreted as being related to the broadening necessary for the electron to tunnel. This point of view shows that conditions for localization are much more favourable away from the centre of the band, where tunnelling is more difficult.

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