

Numerical studies of localization in disordered systems

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Abstract. The results of numerical work on the Anderson model of disordered systems are presented. The sensitivity of the eigenvalues to the choice of periodic or antiperiodic boundary conditions is used as a criterion for localization, and the theory of this criterion is discussed. For the two dimensional square lattice this criterion gives a reasonably sharp result for the onset of localization which is not in conflict with other criteria of localization, and it is found that localization occurs far more easily than Anderson's theory suggests. For the diamond lattice the onset of localization is less sharply defined, and localization occurs less easily than for the square lattice, but more easily than in Anderson's theory.

1. Introduction

Recently, intensive interest has been shown, by physicists working in the field of amorphous semiconductors and other random systems, in the model introduced by Anderson (1958). This model was the first serious attempt at describing quantum mechanical, as opposed to thermal, diffusion of electrons through a random medium.

The Anderson model uses a form of the tight binding approximation in which the wavefunction for an electron moving through a periodic array of sites is taken to be a linear combination of site orbitals with only one orbital considered for each site. The equation for the amplitudes for an eigenstate of energy E is

$$Ea_i = \epsilon_i a_i - V \sum_l a_{i+l} \quad (1.1)$$

where l is a displacement vector ranging over the Z nearest neighbours of site i , V , the coupling, is taken to be some constant between neighbouring sites and zero otherwise, a_i is the amplitude associated with the i th site, and ϵ_i is the energy of the orbital localized on site i . It is assumed that each ϵ_i belongs to a uniform distribution of width W , and is statistically independent of every other site energy. If, for example, the ϵ_i are distributed uniformly in the interval $(-\frac{1}{2}W, \frac{1}{2}W)$ then it is easy to show that the energy band is defined by

$$-\frac{1}{2}W - ZV < E < \frac{1}{2}W + ZV \quad (1.2)$$

Anderson's criterion for the localization of a state is that the imaginary part of the self energy associated with an arbitrary site should be zero with probability unity. For a particular value of the energy E this should occur when the value of W/V exceeds some critical value. The determination of this critical value of W/V involves a complicated statistical argument, and Anderson's (1958) work contains some approximations which

may not be valid (Thouless 1970). There is considerable theoretical haziness concerning the critical value of W/V , and this is one of the reasons for undertaking numerical work. Another reason is that very little is known about the precise nature of the transition.

The numerical work of Khor and Smith (1971) on two dimensional systems suggests that localization, at least in the tail of the band, occurs more readily than Anderson suggests. There is also work by Visscher (1971) that has some bearing on this question. We have studied finite systems in two and three dimensions paying particular attention to the localization condition for the centre of the band. We have also looked for features of the numerical solution which would give some guidance as to the nature of the transition. Two methods of approach are utilized; the first involves a direct study of calculated eigenvectors, and the second depends upon the sensitivity of states to the imposed boundary conditions. This approach has the advantage that only the spectra corresponding to the various boundary conditions used need be calculated; it may also provide a more sensitive test of localization.

2. Criteria for localization

For a sufficiently large system there should be no difficulty in distinguishing between a localized wavefunction, whose amplitude falls off exponentially away from the centre of localization, and a nonlocalized wavefunction extended over the whole system. In practice a numerical study can only be undertaken for a rather small system, and it is important to be able to recognize the occurrence of localization in such a small system.

One measure of localization that has been used in earlier numerical work is the participation ratio (Dean and Bell 1970), or a closely related quantity

$$\alpha = \frac{\sum_{i=1}^N |a_i|^4}{(\sum_{i=1}^N |a_i|^2)^2} \quad (2.1)$$

where the a_i are amplitudes for some particular eigenstate; the participation ratio is essentially $(N\alpha)^{-1}$. This parameter α has its minimum value N^{-1} for a Bloch wave (the participation ratio is unity when all sites participate equally), and has its maximum value, unity, when the wavefunction is completely localized on one site. If the localization is not complete, α^{-1} is of the order of the number of sites over which the peak of the wavefunction is spread. One possible way of studying whether or not states in a particular energy range are localized is to calculate α for different sizes of system. If α tends to a constant value as the size of the system is increased, the states are localized, but if α appears to tend to zero, the states are probably not localized. One difficulty with this procedure, which is a difficulty with all the procedures that we have used, is that random variations of α , from one system to another, obscure systematic dependence of α on the size of the system.

It is only for the lowest state and the highest state in the energy band that α has its minimum value N^{-1} even for a perfect lattice. Other eigenstates are degenerate for the perfect lattice, and numerical evaluation of the eigenfunctions gives real standing waves which are superpositions of Bloch waves. Such standing waves give different values of α according to how they are made up; α could be $\frac{3}{2}N^{-1}$ for a wave with a single set of parallel nodes, or $9/4N$ for a wave with two intersecting sets of nodes, or even $27/8N$ for a wave in three dimensions with three sets of nodal planes. It is reasonable to suppose that for a large system with a small degree of disorder the eigenstates can be regarded as the result

of multiple scattering of Bloch waves, so that the amplitude at a site is due to many waves coming from different scattering centres, and so it should be a random variable with a normal distribution. In that case α should have the value $3N^{-1}$.

We have concentrated on a different criterion for localization. It is clear that the energy of a localized state in a large system should be insensitive to the boundary conditions, provided that the centre of localization is not close to the boundary, since the wavefunction is exponentially small at the distant boundary. Periodic boundary conditions have the advantage that the position of the boundary has no effect, and all sites can be regarded as equally far from the boundary. The procedure we have used is to calculate the energy levels for a particular system using periodic boundary conditions, to repeat the calculation using antiperiodic boundary conditions across one of the boundaries, and then to calculate the difference in energy between corresponding levels when the levels are arranged in order of energy. For strongly localized states the corresponding wavefunctions should be very similar, and the difference in energy should be exponentially small, while for states in an ordered two or three dimensional system there should be little correspondence between the wavefunctions and the energy differences should be comparable with the spacing between levels; for the ordered system the change in boundary conditions produces a change in wavenumber of π/L , where L is the distance across the system, and this produces a change in energy much larger than the spacing between energy levels. The ratio of the energy shift (this difference between corresponding energy levels with the two boundary conditions) to the energy spacing has been used as a measure of the degree of localization. If this ratio decreases as the size of the system is increased the states are localized, but if it does not decrease the states are not localized. It was hoped that this would provide a sharper criterion than the value of α .

There is a rough argument to show what value of this energy shift ΔE to the spacing between energy levels, roughly W/N , gives the condition for localization in a system of N sites. If we take a particular system of N sites and continue it periodically to form an infinite periodic system with the original system of N sites as a unit cell, the continued system will have energy levels in N energy bands of width $d\Delta E$, where d is the dimensionality of the system. The quantity $\frac{1}{2}\Delta E$ can therefore be regarded as the strength of the coupling between states on neighbouring cells. The problem we would like to be able to solve is the problem in which these large unit cells are not identical, but are randomly chosen from the same population. The coupling between these cells has a strength of order $\frac{1}{2}\Delta E$, variation in energy of states of similar character from one cell to another is of order W/N , and so our new problem is like the old problem with V/W replaced by $\frac{1}{2}N\Delta E/W$. If this parameter is less than the original one, it should become even less if we could repeat the argument one stage further, making cells of cells, and so on. Our tentative criterion for localization is therefore

$$\text{or } \frac{V}{W} > \frac{N\Delta E}{2W}$$

$$N\Delta E < 2V \tag{2.2}$$

The numerical constant should not be taken seriously.

In the Appendix perturbation theory is used to derive a relation between the ratio of the shift ΔE to the spacing η between energy levels and the mean free path λ in the case of a relatively small degree of disorder. This derivation makes use of an assumption that the matrix elements of the momentum operator between two states do not depend strongly on the difference in energy between the two states, and this assumption may not

be correct. The results are that

$$\frac{\Delta E}{\eta} \simeq \frac{\lambda k}{\pi} \quad (2.3)$$

in two dimensions, and

$$\frac{\Delta E}{\eta} \simeq \frac{2\lambda Lk^2}{3\pi^2} \quad (2.4)$$

in three dimensions, where k is the wavenumber and L is the length of the system. In both cases the shift is proportional to the mean free path, but in two dimensions the ratio is independent of the size of the system, while in three dimensions it increases with the size of the system. These results can be taken as an indication of conditions in which the shift is comparable with the spacing. The use of perturbation theory is invalid when this ratio is of the order of unity—the actual shifts can never be appreciably larger than the spacing. Perturbation theory diverges when levels attempt to cross, and we could not detect any crossing, since levels are identified only by the order in which they occur.

3. Methods of calculation

Particular systems described by an equation of the form of equation 1.1 were set up and the eigenvalues found numerically. The lattices studied were the two dimensional square lattice, and the three dimensional diamond lattice. There were two reasons for choosing the diamond lattice. One reason is that the coordination number is the same as that of the square lattice, and so differences between them are likely to be due to dimensionality rather than to different connectivity; it is the connectivity which is important in Anderson's (1958) work. A second reason for choosing the diamond lattice is that for a given number of sites the boundary conditions appear to be less important for a diamond lattice than for other lattices. One measure of the effect of periodic or antiperiodic boundary conditions is the least number of steps which a path starting from a given point and ending at the same point can have if the path crosses the boundary once; this determines the lowest moment of the hamiltonian whose trace is affected by the boundary condition. For a diamond lattice of 216 sites the shortest path of this sort has 12 steps, while for the same size of simple cubic lattice the shortest path would have 6 steps.

For each lattice various sizes were studied. For the square lattice the number of sites varied from 9 to 100, while for the diamond lattice 8, 64 and 216 sites were used. For a given kind and size N of lattice, site energies ϵ_i were determined by assigning the integers from 1 to N to the N sites in a random manner. If the number assigned to the site i was n_i , the site energy was taken to be $-n_i W / (N - 1)$. The eigenvalues were calculated for the different values of W using the same numbers n_i , so that the calculated dependence of various quantities on W is subject to less statistical error than the dependence on N is subject to.

For all the systems studied the complete set of eigenvalues was found using a subroutine based on the Householder method, written for the KDF 9 computer by Dr R E Borland of the National Physical Laboratory; this method gives very precise values for the eigenvalues. The eigenvalues were calculated both for periodic boundary conditions and for boundary conditions which were antiperiodic across one boundary—it might have been better to use antiperiodic boundary conditions on all boundaries instead of on only one boundary. In some cases some or all of the eigenvectors were calculated. With the

routine used it was quicker to calculate the eigenvalues for both boundary conditions than the eigenvectors for a single boundary condition.

The value of V was taken to be unity, and W varied between 0 and 25.

The eigenvalues were arranged in ascending order, and the differences ΔE between corresponding eigenvalues for the two boundary conditions were calculated. Since these differences varied by many orders of magnitude for each system, as can be seen from figure 2, the geometric mean $\overline{\Delta E}$ of the N differences was calculated as a measure of the typical magnitude. This geometric mean is indeed a typical value of the energy shift, as it comes close to the peak of the probability distributions seen on this and similar figures. By using $\overline{\Delta E}$ for the whole band we lose the possibility of distinguishing regions of localized and nonlocalized states within the band, and of finding a mobility edge between the two regions. If the density of states had varied more through the band it might have been possible to find the mobility edge by studying the systematic variation in ΔE through the band, but in fact the random variation of ΔE masks any systematic effects in the cases we have studied.

The quantity α defined by equation 2.1 was calculated in some cases so that its behaviour could be studied. This is the quantity which has been used in the work of Visscher (1971).

4. Results

4.1. Two dimensional square lattice

Figures 1a and 1b are coarse histograms of the densities of states for the $N = 100$, $W = 5$, square lattice, and $N = 216$, $W = 15$, diamond lattice problems respectively. The W values in each case correspond to the regions in which we find that the transition from localized to nonlocalized states occurs. It appears that the singularities associated with the densities of states in the $W = 0$ case have been smoothed out in both cases.

As can be seen from the histograms shown in figure 2, the energy shifts calculated for given values of N and W are spread over many orders of magnitude. There is a slight tendency for states at the extreme ends of the band to have lower values of ΔE than the other states, and those states which are unusually close to one another in energy have unusually large values of ΔE , but otherwise the variation of ΔE through the band appears to be random rather than systematic. Other measures of the degree of localization also vary in an irregular manner from one level to another. For this reason we have concentrated attention on the geometric mean $\overline{\Delta E}$ of all the energy shifts, rather than on the behaviour in any particular part of the energy band.

In figure 3 $N\overline{\Delta E}$ is plotted as a function of W for various values of N , while in figure 4 the same quantity is shown as a function of N for various values of W . The most striking result is that Anderson's (1958) estimate for the critical value of W/V for the square lattice is much too high. If we take the value 2.64 which Shante and Kirkpatrick (1971) quote for the connective constant K of the square lattice, Anderson's critical value of W/V is about 30. Even for $W/V = 20$ the mean shift is very small and decreasing rapidly as the size of the system increases; by any other criterion all the states are strongly localized for this value of the ratio.

For the larger values of N the behaviour of $N\overline{\Delta E}$ as a function of N and W is sufficiently smooth that little advantage seemed likely to be gained by studying slightly larger systems, although a value of N as high as 225 could have been handled without any change in the procedure.

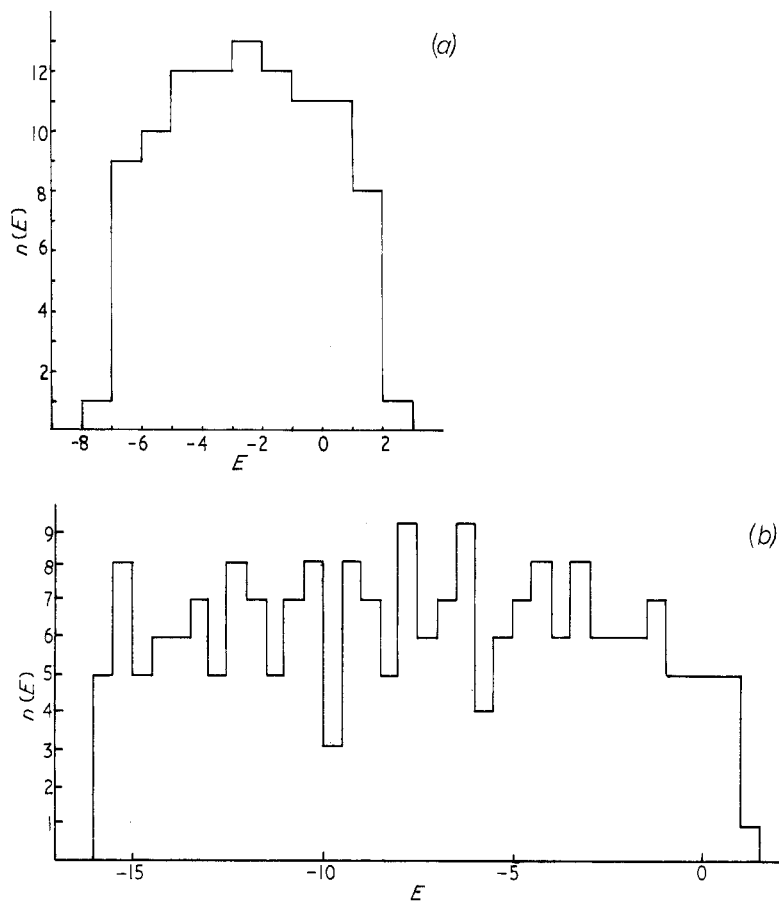


Figure 1. Histograms of the density of states for (a) the $N = 100$, $W = 5$, square lattice problem, and (b) the $N = 216$, $W = 15$, diamond lattice problem.

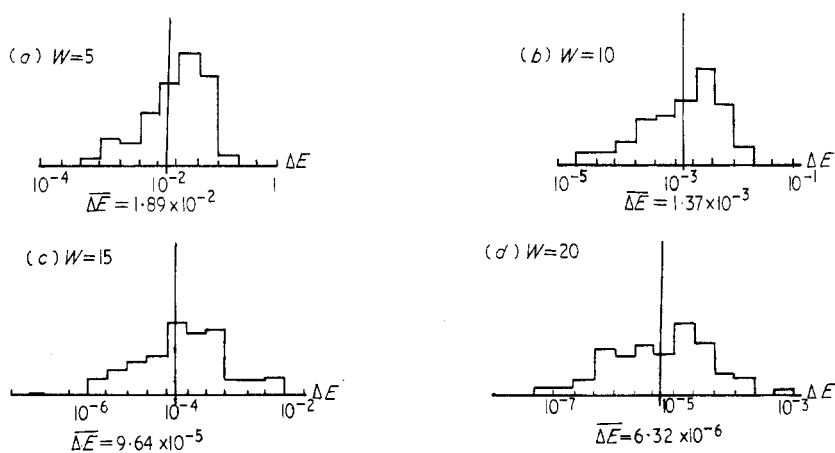


Figure 2. Energy difference histograms in the $N = 100$, square lattice problem for (a) $W = 5$, (b) $W = 10$, (c) $W = 15$, (d) $W = 20$. In each case the vertical line refers to the position of the geometric mean $\overline{\Delta E}$.

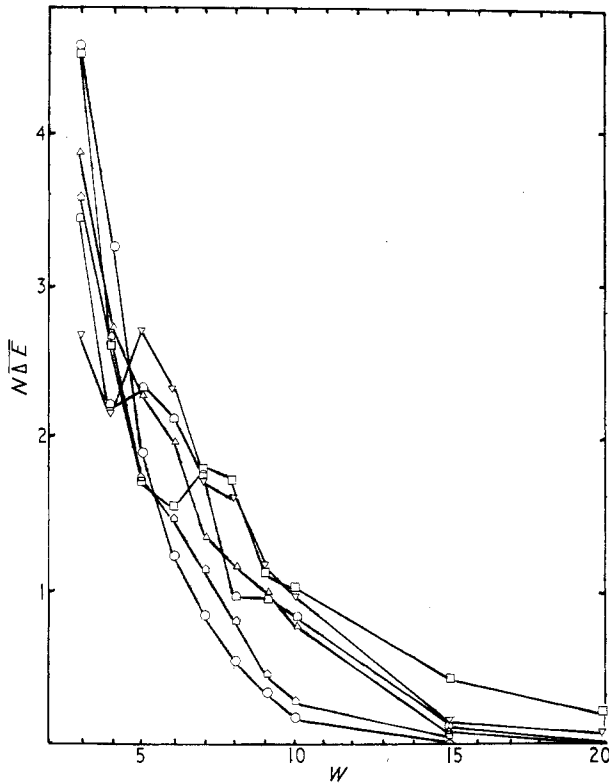


Figure 3. $N\overline{\Delta E}$ against W plots for square Anderson systems of various sizes for the following values of N : \square 25, ∇ 36, \triangle 49, \square 64, \triangle 81, \circ 100.

For the lowest values of W shown here, which are 3, 4 and 5, the quantity $N\overline{\Delta E}$ seems to vary with N in an unsystematic manner, but seems to have a larger value for the lower value of W . This is in rough agreement with equation 2.3 if the mean free path λ is taken to be of the order of the interatomic spacing. For W equal to 8 or more $N\overline{\Delta E}$ goes down steadily and rapidly as the size of the system is increased. For slightly smaller values of W the decrease does not become apparent until N exceeds 64, presumably because the localization distance is large in these cases.

From these two figures it looks as if the critical ratio of W/V is between 5 and 6. This may be an overestimate, since it may be that a larger system would show a region of W in which localization occurs with a localization distance larger than the systems studied here. This result is in agreement with the work of Khor and Smith (1971) who have shown clear evidence of localization for W/V equal to 6.4. If our estimate is correct, the lowest value of $N\overline{\Delta E}$ for nonlocalized states is somewhat less than 2, in good agreement with equation 2.2.

In figure 5 the behaviour of the parameter α , defined by equation 2.1, is shown as a function of W for various energy levels close to the bottom of the band, in the case $N = 100$, with antiperiodic boundary conditions. For W greater than 3 the eigenstates associated with corresponding energy levels for the two kinds of boundary conditions closely resemble each other, in the cases we have examined in detail. One thing that should be noticed is that α increases earlier for the ground state than for other states, although its value for $W = 0$ is less than that of the other states. Beyond $W = 8$ or so, the value of α

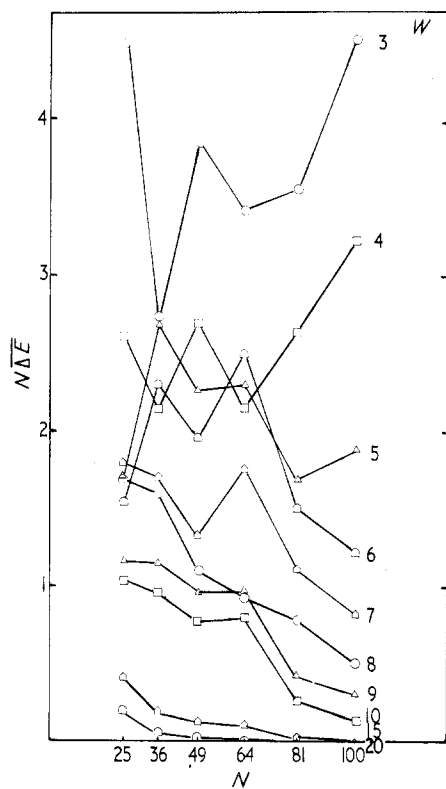


Figure 4. $N\Delta E$ against N plots for values of W ranging from 3 to 20 for the square lattice problem.

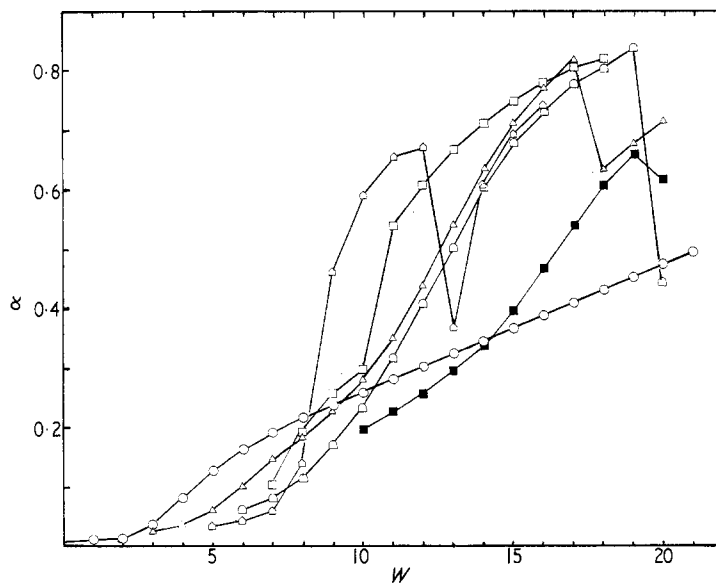


Figure 5. α against W plots for states \circ 1, \triangle 2, \blacksquare 3, \triangle 5, \square 6, \triangle 10 of $N = 100$ square lattice spectrum, with antiperiodic boundary conditions.

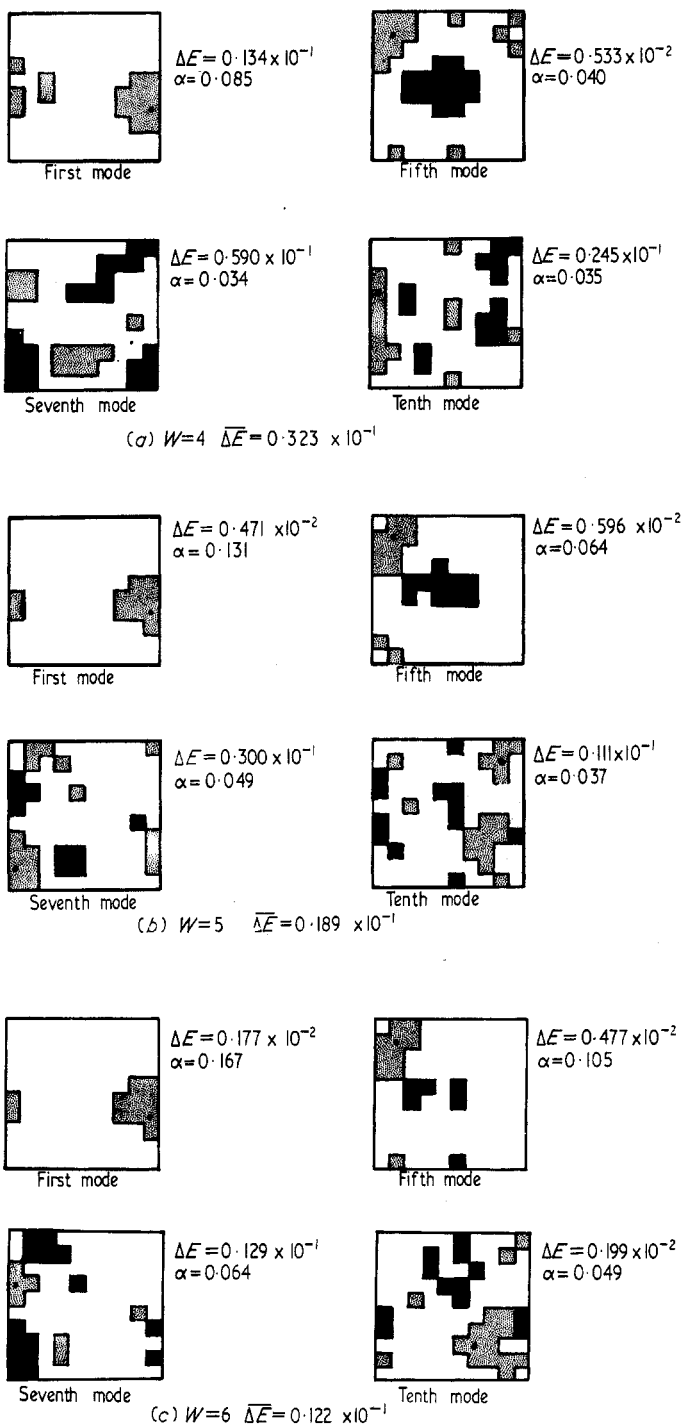


Figure 6. Amplitude contour plots for the $N = 100$ square lattice problem for (a) $W = 4$, (b) $W = 5$, and (c) $W = 6$. The two kinds of shading refer to the sign of the amplitude, and the dot gives the position of the amplitude whose magnitude is greatest. Periodic boundary conditions were used across both boundaries.

is, to a very good approximation, a linear function of W . For the other states α retains a small value, gently increasing with W , and then increases by a factor of five or so in the range of W from 5 to 8. Different states vary quite a lot from one another. There are some sudden changes of α than can be seen, for example, in the sixth and tenth modes in this figure. These are due to two modes coming close to one another in energy, so that the eigenstates cease to be localized in a single region, but are superpositions of states localized in two different regions. This results in a value of α which may be reduced by a factor of 2, and also results in much larger values of ΔE .

For small values of W , of the order of 2 or 3, the value of α for states other than the ground state does not differ much from the theoretical value of $3N^{-1}$, which is 0.03. For example, for $W = 3$ the lowest five states give values of α equal to 0.038, 0.031, 0.036, 0.025, 0.025; the first figure referring to the ground state.

The results shown here seem to be compatible with localization setting in for most states in a range of W from 5 to 6.

Figure 6 shows a series of crude contour plots for the system with $N = 100$ in this range of W . The shaded squares correspond to sites where the amplitude is greater than its root mean square value of 0.1. The different sorts of shading are to show the sign of the amplitude, and a dot is drawn to show the site with the largest amplitude. The boundary conditions are periodic in both directions, and so the position of the boundary shown in the figure is of no significance.

For the lowest state the sites where the amplitude is large are already concentrated in one region for $W = 4$, while the other states have sites of large amplitude scattered over the system. For $W = 5$ a slight tendency of the large-amplitude sites to be clustered in a portion of the system is detectable for the fifth and seventh modes, which is clear for $W = 6$. The tenth mode shows only slight signs of a tendency to localize for $W = 6$.

It should be emphasized that regions in which the amplitude is large are not regions in which the site energy is particularly close to the energy of the state, although the site at which the maximum amplitude occurs generally is a site whose energy is close to the energy of the state. States close together in energy will be localized in different regions of the system.

4.2. *Diamond lattice*

Some numerical calculations were made also for the diamond lattice. The connective constant for this lattice is 2.88 (Shante and Kirkpatrick 1971), and so, according to Anderson's (1958) theory the critical value of W/V should be only a little greater than that for the square lattice.

Calculations of the energy shifts due to the change from periodic boundary conditions to conditions antiperiodic across one boundary were made for the cases $N = 8$, $N = 64$ and $N = 216$, with varying values of W . The method used was the same as for the case of the square lattice. The results are shown in figure 7.

The following features can be seen in this diagram.

(i) For W less than about 5 the values of $N\Delta\bar{E}$ are rapidly decreasing functions of W , and they are much larger than the corresponding values for the square lattice. In accordance with equation 2.5, the value of $N\Delta\bar{E}$ is larger for larger values of N .

(ii) There is a range of W from about 5 to 12 or more in which the value of $N\Delta\bar{E}$ declines slowly from about 5 to about 2 or 1 and is more or less independent of N .

(iii) For values of W larger than 15 the value of $N\Delta\bar{E}$ falls fairly rapidly for large N ,

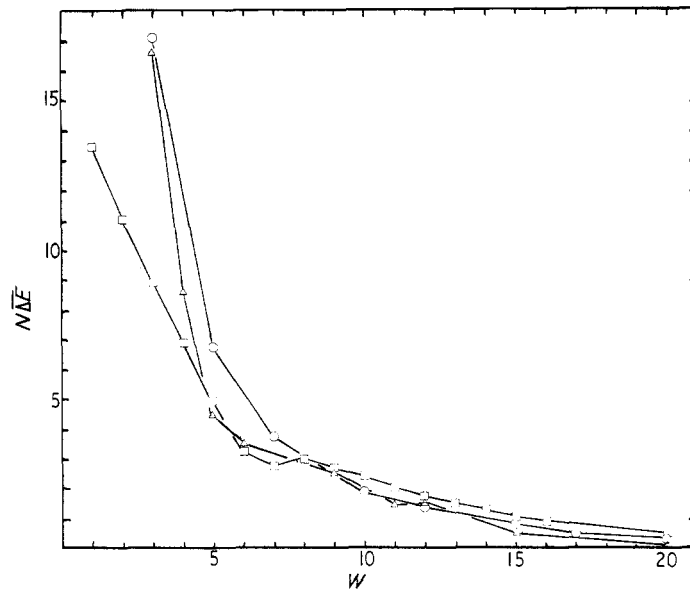


Figure 7. $N\overline{\Delta E}$ against W plots for the diamond lattice problem. The systems considered consisted of \square 8, \circ 64 and \triangle 216 sites.

less rapidly for smaller N . It does not fall so rapidly as it does for the two dimensional case.

The first of these regions is clearly a region in which nonlocalized states exist, and the apparent correctness of equation 2.4 suggests that the model of plane wave states coupled by the random scattering is applicable.

In the third region there is clearly localization, since $N\overline{\Delta E}$ is a decreasing function of N .

We have no theory to explain the behaviour of $N\overline{\Delta E}$ in the second region, if it is real and not just a chance result of our small system. It is tempting to identify this with Cohen's (1970) region of electronic Brownian motion, but we have no information on this beyond what has been presented here, since we have not calculated eigenstates for the diamond lattice. The value of $N\overline{\Delta E}$ at the end of this region is of the order of magnitude predicted by equation 2.2.

5. Conclusions

The calculations of the effect of boundary conditions on the energy levels provide clear evidence for a transition from extended to localized states in the square lattice at a value of W/V of the order of 5 or 6, which is less than that predicted by Anderson (1958) by a factor of five. This method provides a sensitive test of localization, but does not disagree with other tests of localization.

The three dimensional results suggest a critical value of W/V larger by a factor of two or more, but the transition is less clear than in the two dimensional case. There may exist an intermediate region in which the states are not localized, but not adequately described in terms of weakly coupled plane waves.

It is interesting to note that these numerical results agree better with the simpler, but probably incorrect, versions of Anderson's argument (Ziman 1969, Thouless 1970,

Herbert and Jones 1971, Economou and Cohen 1971) that have been published recently than with the more complicated original version. The difference between two and three dimensional results is not, however, a consequence of any of these arguments.

Acknowledgments

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Appendix

We derive here an expression for the effect of a change in boundary conditions from periodic for a system with period L to the more general form in which the amplitude changes by a factor $\exp(iKL)$ when the coordinate x is increased by the period L . If K is a multiple of $2\pi/L$, periodic boundary conditions are recovered, and if K is an odd multiple of π/L , antiperiodic boundary conditions are obtained.

This change in boundary conditions is equivalent to a transformation to a moving frame of reference, or to a gauge transformation, and a solution of the Schrödinger equation can be written in the form

$$\psi(\mathbf{r}) = \phi(\mathbf{r}) \exp(iKx) \quad (\text{A.1})$$

where ϕ satisfies periodic boundary conditions and satisfies the Schrödinger equation with additional terms

$$\left(\frac{\hbar K}{m}\right) \hat{p}_x + \left(\frac{\hbar^2 K^2}{2m}\right) \quad (\text{A.2})$$

in the hamiltonian. For the lattice problem the momentum operator \hat{p}_x must be replaced by the corresponding difference operator, the mass m must be replaced by Vl^2/\hbar^2 where l is the lattice spacing (for a square or simple cubic lattice), and the term $\hbar^2 K^2/2m$ is replaced by an operator with matrix elements equal to $\frac{1}{2}VK^2l^2$.

The operator \hat{p}_x has no diagonal matrix elements between the real eigenstates of the original problem with periodic boundary conditions ($K = 0$). The energy shift is therefore given to second order in K as

$$\Delta E_i = \frac{\hbar^2 K^2}{m^2} \sum_j \frac{|(\hat{p}_x)_{ij}|^2}{E_i - E_j} + \frac{\hbar^2 K^2}{2m} \quad (\text{A.3})$$

It can be shown that this expression differs from zero only because of fluctuations in the value of the sum, and these fluctuations are dominated by small values of $|E_i - E_j|$. From the Kubo formula it can be shown that the sum is proportional to the contribution of the level i to the integral of the conductivity, and this cancels with the second term on the right, in so far as the Thomas–Reiche–Kuhn sum rule is satisfied.

For localized states $[\hat{p}_x]_{ij}$ is proportional to $\hat{x}_{ij}(E_i - E_j)$ and the expression on the right of equation A.3 is identically zero, apart from some exponentially small terms which

arise from the fact that the operator \hat{x} is not properly defined with periodic boundary conditions.

In the case of nonlocalized states we can compare this expression with the Kubo–Greenwood formula for the electrical conductivity of a cube of side L , which is

$$\sigma = \frac{2\pi e^2 \hbar L^3}{m^2} |[\hat{p}_x]_{ij}|_{\text{av}}^2 [N(E)]^2 \quad (\text{A.4})$$

in the form given by Mott (1970), where $N(E)$ is the density of states per unit volume at the Fermi surface. In order to get an expression which can be compared with the result of the Boltzmann equation it is necessary, as Mott has emphasized, to assume that the mean square value of the matrix element $[\hat{p}_x]_{ij}$ evaluated between eigenstates of the system, does not depend strongly on the energy difference $E_i - E_j$ between the eigenstates.

If this assumption of the independence of the matrix element of \hat{p}_x from $E_i - E_j$ is correct even for spacings as small as typical spacings between energy levels of the entire system—and it should be emphasized that the finite value of the conductivity given by the Kubo–Greenwood formula in the DC limit depends only on this assumption being true for $E_i - E_j$ of order $\hbar\omega$, where ω is a small AC frequency—then the magnitude of the square matrix element in equation A.3 can be taken from equation A.4. The sum over states, which is a sum over positive and negative terms, is likely to be dominated by the largest term, which is of the order of one over the spacing between energy levels, or $L^3 N(E)$. A more precise value can be obtained if it is assumed that the energy levels are uncorrelated, in which case the value of the sum has a Cauchy distribution whose width is π times this quantity. The geometric mean of the energy shift is therefore given by

$$\overline{\Delta E}_i = \frac{\pi \hbar^2 K^2 L^3 N(E)}{m^2} |[\hat{p}_x]_{ij}|_{\text{av}}^2 = \frac{\sigma \hbar K^2 L^3}{2e^2} \eta \quad (\text{A.5})$$

where η is the level spacing.

Finally we can express the conductivity in terms of the mean free path λ as

$$\sigma = \frac{e^2 k^2 \lambda}{3\pi^2 \hbar} \quad (\text{A.6})$$

so that we have

$$\frac{\overline{\Delta E}_i}{\eta} = \frac{k^2 K^2 L^3 \lambda}{6\pi^2} \quad (\text{A.7})$$

For antiperiodic boundary conditions KL is equal to π , but the shift is a periodic function of KL with period 2π , so substitution of KL equal to π in this expression probably overestimates the shift; it may be better to put KL equal to 2. With this substitution we get

$$\frac{\overline{\Delta E}_i}{\eta} \simeq \frac{2k^2 L \lambda}{3\pi^2} \quad (\text{A.8})$$

A similar calculation in the two dimensional case gives

$$\frac{\overline{\Delta E}_i}{\eta} = \frac{k\lambda K^2 L^2}{4\pi} \simeq \frac{k\lambda}{\pi} \quad (\text{A.9})$$

It is interesting to note that in the two dimensional case the numerical results show that $\overline{\Delta E}_i/\eta$ is of order $\frac{1}{3}$, where the transition to localized states occurs, and so $k\lambda \simeq 1$; the mean free path is therefore of the order of the interatomic spacing at the mobility edge.

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