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# A nearly exact method of solving certain localisation problems 

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#### Abstract

The old theories of localisation of Anderson and Abou-Chacra et al are reexamined. It is argued that ( $a$ ) the convergence properties of the renormalised perturbation series for the self-energy are predominantly governed by its first term; and (b) the localisation problem in a real lattice can be mapped on to the localisation problem in a Cayley tree lattice in which the non-contributing branches are trimmed off. The connectivity constant for the trimmed Cayley tree, which can be evaluated exactly, should be used in the AbouChacra et al method to obtain results for a real lattice. Calculations for two-dimensional lattices show partial agreement with the well known result that all states should be localised at any disorder-the triangular lattice (coordination number $C=6$ ) appears to show complete localisation only above a critical value of disorder, the honeycomb lattice ( $C=3$ ) shows complete localisation always, and the square lattice $(C=4)$ is found to be the marginal case.


## 1. Introduction

Despite the phenomenal success of Anderson's (1958) idea of electron localisation in a medium of random potential the embarrassing truth remains that both the old and the new theories (for a review see Lee and Ramakrishnan 1985) have by and large not been able to answer satisfactorily the simple questions such as where will the mobility edges be for a given system; what will be the critical amount of disorder, say $W_{c}$, to cause the Anderson transition (Mott and Davis 1979), etc, even for simple model systems. The only saviours have been the numerical simulations of Licciardello and Thouless (1978), Weaire and Srivastava (1977), and many others including recent ones like Elyutin et al (1984) and Schreiber (1987). In order to find quantitative answers to such questions for realistic systems if we scrutinise the available theories we find that Anderson's original theory (Anderson 1958) and the self-consistent theory of Abou-Chacra et al (1973) are still the most rigorous although their estimates are too high compared with the simulation results. The reason for the disagreement, we suggest, is that the connectivity constants for the realistic systems used in the analytical theories (Anderson 1958, Abou-Chacra et al 1973, hereafter called AAT) were much too high.

We have re-examined the Anderson-Thouless theories and have obtained an exact method for calculating the connectivity constant for the hierarchy of closed self-avoiding random walks (SAWs) that are pertinent to the localisation problems in a given lattice.

[^0]This enables us to handle the localisation problems in real systems almost exactly within the Anderson's tight-binding model (Anderson 1958).

Anderson (1958) and AAT (1973) studied the convergence of a renormalised perturbation series (RPS) for self-energy $S_{i}$ on site $i$,

$$
\begin{equation*}
S_{i}(Z)=\sum_{j \neq i}\left(V_{i j} g_{j}^{i} V_{j i}+\sum_{k \neq i, j} V_{i j} g_{j}^{i} V_{j k} g_{k}^{i, j} V_{k i}+\ldots\right) \tag{1}
\end{equation*}
$$

where $g_{n}^{i, j, \ldots, m}=\left(Z-e_{n}-S_{n}^{i, j, \ldots m}\right)^{-1}$ is the Green function; $e_{n}$ is the site energy on site $n$ and is distributed randomly over the lattice sites; $V_{n m}$ is the transfer integral between the nearest-neighbour sites $n$ and $m$ and takes a fixed non-random value, say $V$; the superscripts denote the sites excluded once they are traversed in the course of a random walk, so only the SAWs contribute to (1). For the localised states the RPS (1) converges and is defined term by term. Since for the localised states $\operatorname{Im} S_{i} \rightarrow 0$ as $\operatorname{Im} Z \rightarrow 0$ such that $\operatorname{Im} S_{i} / \operatorname{Im} Z$ remains finite for $\operatorname{Im} Z \rightarrow 0$, the Rps for $\operatorname{Re} S_{i}$ and for $\operatorname{Im} S_{i} / \operatorname{Im} Z$ should converge simultaneously (Im and Re represent the imaginary and real parts respectively). More explicitly, writing $S_{i}=R_{i}+\mathrm{i} \Delta_{i}$ and $Z=E \pm \mathrm{is}$, we demand that

$$
\begin{align*}
R_{i} & =\sum_{j \neq i} V^{2} / a_{j}^{i}\left(1+\sum_{k \neq i, j} V / a_{k}^{i, j}(1+\ldots)\right) \quad a_{n}^{i, j, \ldots, m}  \tag{2a}\\
& =E-e_{n}-R_{n}^{i, j, \ldots, m}
\end{align*}
$$

and
$\lim _{s \rightarrow 0} \Delta_{i} / s \equiv \Delta_{i}^{\prime}=\sum_{j \neq i} \frac{V^{2}\left(1+\Delta_{j}^{i \prime}\right)}{\left(a_{j}^{i}\right)^{2}}\left[1+\sum_{k \neq i, j} \frac{V}{a_{k}^{i, j}}\left(1+\frac{\left(1+\Delta_{k}^{i, j}\right) /\left(1+\Delta_{j}^{i \prime}\right)}{a_{k}^{i j} / a_{j}^{i}}\right)(1+\ldots)\right]$
should converge at the same time. The perturbation theory is done for large disorder $W$ (measured as the width of the distribution function for $e_{n}$ ), where $W \gg V$.

Assuming that (i) the probability distribution of individual terms of the RPS has a large tail, (ii) all denominators $<4 V^{2} / W$ should be ignored for $E=0$, and (iii) each of the $K^{n}$ paths of $n$ steps ( $K$ being the connectivity constant for the lattice) from a point makes a contribution that is statistically independent of the contributions from the others, Anderson gave the following condition for the localisation of the band centre,

$$
\begin{equation*}
W>4 K V \ln (W / 2 V) \tag{3}
\end{equation*}
$$

Surprisingly, AAT (1973) found exactly the same condition (3) in a self-consistent treatment of localisation (at the band centre). Their treatment is exact for a Cayley tree (CT) of connectivity $K$ and involves only the two-step diagrams in (2), which amounts to ignoring all the terms except the first one in ( $2 a$ and $b$ ). We focus our attention on this coincidence to examine the significance of the statistical independence (or otherwise) of SAWs in arriving at condition (3).

In § 2 we discuss the question of statistical independence and, having settled it, we enquire in § 3 why the Anderson-Thouless-type approaches do not yield results in agreement with the numerical results. The answer, it is argued, is related to the 'proper' connectivity constant that should be used in the Anderson-Thouless approaches. The quest for this leads us to the construction of a trimmed ct exactly equivalent to a given real lattice for the purposes of localisation studies. This is done in $\S 4$. Localisation in the trimmed CT is studied in $\S 5$ and a surprising finding is discussed in $\S 6$.

## 2. The question of statistical independence of saws

While Anderson's assumptions (i) and (ii) are generally believed to be reasonable, assumption (iii) has been criticised (Thouless 1970, Economou and Cohen 1972) and it is often felt that this makes his treatment equivalent to that of a CT. The basis of the criticism has been that different SAws in a real lattice have many sites in common and therefore should not be treated as statistically independent. This is perfectly valid, but we argue that this is not the reason that makes Anderson's treatment equivalent to that of the CT, for in the CT too the SAWs have sites in common.

In a CT the number of new options for the next step after the $n$th step is $K^{n}$, and they are all treated as independent of each other; this is also true in a real lattice where all the new steps are, quite justifiably, independent of each other. Thus, so far as the statistics of new steps at a given stage of a SAW is concerned, both the CT and the real lattices behave similarly; also the $n$-step SAWs are not statistically independent of each other in either the CT or the real lattices. Despite these similarities in behaviour, the SAWs in the two types of lattices are intrinsically different in that the real lattices have $n$ step closed sAws (i.e., those that interest us in connection with the RPs (1)) and the CT has two-step open SAWs of length $n$; in real lattices only the first term of the RPS has twostep saws. With this distinction emphasised, it is easy to appreciate the coincidence pertaining to condition (3)-while Anderson investigates the contributions from the higher terms in (2) within the approximation scheme (i)-(iii), in the СТ approximation of AAT all the higher terms are completely ignored and one concentrates only on the first term in (2). Yet the end result, namely condition (3), is the same.

It is hard to expect that as a consequence of the 'statistical independence' all the higher terms in (2) cancel each other leaving the non-zero contribution to come from the first term alone and thus reducing the problem to become exactly equivalent to the localisation in the ст. The only plausible explanation seems to be that the question of statistical dependence or otherwise of the terms within the square brackets in the series (2) is not important and that the dominant contribution comes from the first term alone. Thus, only the two-step saws of the first term govern the convergence or divergence of the infinite series (2).

This is also indirectly indicated by the fact that localisation in a CT is more difficult than in a real lattice of the same $K$ because a ct has many more avenues to let an electron diffuse away. Thus, if an eigenstate is localised on a CT, a state of the same energy is expected to be localised in the real lattice of the same $K$. While in understanding this argument one should be a little cautious and bear in mind that a СT of connectivity $K$ is not exactly represented by the first term of the RPS for a real lattice of coordination number $C(=K+1)$. The first term of the RPS represents a tree structure of connectivity less than $K$. However, since its branches are non-intersecting it also offers more avenues to diffuse away than those existing in the real lattice represented by the full RPS.

So, in principle, it seems it should be sufficient to concentrate on the first term of the RPS and the convergence properties of the continued fraction in it to study the localisation in a real lattice. Since the first term can be studied exactly as was done by AAT, the results should be more or less exact for the real lattice. But we know that this is not the case and that the results obtained by Anderson (1958) as well as those by AAT for $W_{\mathrm{c}}$ are nowhere near the numerical estimates. The answer to this anomaly can be that the connectivity constants used in both these calculations were not the right ones and were always too high.




Figure 1. Sequences of steps taken in self-avoiding manner on a square lattice: solid lines show the paths chosen by the walker and the broken lines show the possibilities available for the next step. The numbers denote the branch indices: the possibilities for the walker to step to the right, straight ahead or left are indicated by 1,2 and 3 , respectively. Any direction could be chosen for the first step off the origin. Suppose he chooses to go to site 1 , paths in all other three directions evolve in identical fashion. All possible saws shown on the left have been put together in the form of non-intersecting branches emanating from the origin. Note that the points on the resulting Cayley tree ( $\bigcirc \bigcirc$ ) denote the stages at which branches are missing respectively due to the origin and the site next to it popping up on the way. The procedure can be continued indefinitely. The result will be an infinite Cayley tree with many missing branches.

## 3. Proper connectivity constant

The connectivity constant for a given lattice is calculated from

$$
\begin{equation*}
K=\exp \left[\lim _{n \rightarrow \infty}\left(\ln S_{n}\right) / n\right] \tag{4}
\end{equation*}
$$

where $S_{n}$ is the number of SAws of $n$ steps in the lattice. The value of $K$ is always less than $K=C-1$, where $C$ is the coordination number for the lattice. The calculations using $K$ in place of $K$ have yielded better results (e.g., Brouers and Kumar 1975), but we show that it is not good enough (in fact it is even wrong) to replace $K$ in the cт calculation with $\boldsymbol{K}$. The CT that actually corresponds to a given real lattice for localisation studies is in fact a section of the cT of non-integral connectivity $K$-we will call it a trimmed Cayley tree (T-CT) of connectivity constant $k(k<K<K)$, which we will determine exactly in the following.

First let us construct the CT of connectivity $\boldsymbol{K}$ corresponding to a given real lattice and compare it with a full CT of connectivity $K$. Then we can easily work out which section of the $K$ CT actually interests us.

The process of constructing the $K$ CT corresponding to a square lattice is shown in figure 1. Starting from an arbitrary origin a random walker can take the first step in four possible directions. These form the first four branches of the desired CT. In whatever
direction the random walker goes it will have three possible directions in which to take the next step, so we add three branches to each of the first four branches. On the tip of each of these two-step saws we examine the number of new steps that can be taken such that the walker does not step on any of the previous two sites it has traversed. These new possibilities are added as new branches. Progressing in this manner, at an arbitrary stage $n$ we look at the tip of each of the $n$-step SAWs individually and independently of each other, and count the number of new steps that can be taken without leading to any of the previous $n$ sites already covered in that particular SAW. These possible new steps are added at the top as new branches. Monitoring the branching and progress of each SAW we construct a tree of all possible SAWs that can be performed on a real lattice. This will be a CT embedded in an infinite-dimensional space, but note that compared with a full CT that has the same number of branches (i.e., $C-1$ ) at each joint, this CT has far fewer branches; many branches go missing (in a seemingly random manner) because of the self-avoiding nature of the random walk on the lattice. From an arbitrary site on a SAW the number of new options to step forward can range from 0 to $(C-1)$. In the asymptotic limit, $n \rightarrow \infty$, if we calculate the connectivity constant for this CT we will simply get the result $K$ according to
$K=$ number of new sites to which a given site is connected

$$
\begin{aligned}
& =\lim _{n \rightarrow \infty} S_{n+1} / S_{n} \\
& =\exp \left[\lim _{n \rightarrow \infty}\left(\ln S_{n}\right) / n\right] .
\end{aligned}
$$

Even the $\boldsymbol{K}$ Ст has many more branches than those of interest to us, as we show in § 4.

## 4. The trimmed Cayley tree

In a given real lattice the SAWs that contribute to the RPS (1) or (2) constitute a hierarchy. Each term of the RPS is represented by a set of SAWs of fixed length that originate and terminate at the arbitrary origin. For convenience call them SAWs ${ }^{(1)}$. Since each term can also be expanded as a continued fraction, we find that after the first iteration of the expansion process the denominator consists of all the saws that originate and terminate on the sites traversed by the SAWs ${ }^{(1)}$. Call them SAWs ${ }^{(2)}$. At the next iteration stage the denominators consist of all the SAWs originating and terminating at the sites covered by the SAWs ${ }^{(2)}$. Thus we find that the RPS is actually represented by a whole hierarchy of the sAWs as is also illustrated by a diagram by Srivastava and Chaturvedi (1982).

The above hierarchy of closed SAWs for a given real lattice will be represented in the $K$ CT by those branches that are able to reach up to a point (or joint) in the tree where the connectivity is less than $K(=C-1)$, but are unable to grow further. Take, for example, $C=4$ (i.e., $K=3$ ), then at a joint $n$ steps away from the origin, suppose the new step can be taken only in one of the three directions and the remaining two directions are blocked because they lead to the sites already traversed. At this joint, these two blocked $(n+1)$-step saws are actually of interest to us. Some of the missing branches of this type at stage $n$ are shown schematically in figure 2 as dotted lines. We can isolate two kinds of joints at stage $n:(a)$ where the connectivity to the $(n+1)$ th stage is $K$, and (b) where it is $<K$, say, $K^{\prime}$. Out of a total number, $S_{n}$, of saws reaching up to stage $n$, $M_{n}$ lead to joints of type (b). In the limit $n \rightarrow \infty$ we are interested in the connectivity, $\boldsymbol{k}$, of the dotted lines, which may be viewed as 'stumps' of the missing branches sticking


Figure 2. Schematic representation of the $n$th stage of a $C T$ with $K=3$. The solid dots represent sites with connectivity $K$ and those with connectivity $K^{\prime}(<K)$ are shown by circles. Of the total number $S_{n}$ of the sites, $M_{n}$ are circles.
out of the $M_{n}$ sites. It is straightforward to write the following relation between $S_{n}, M_{n}$, $K$ and $K^{\prime}$,

$$
\begin{equation*}
K\left(S_{n}-M_{n}\right)+K^{\prime} M_{n}=S_{n+1} \tag{5}
\end{equation*}
$$

Using the fact that $S_{n+1} / S_{n}=K$, we obtain $K^{\prime}$ as

$$
\begin{equation*}
K^{\prime}=K-(K-K) S_{n} / M_{n} \tag{6}
\end{equation*}
$$

Then $\boldsymbol{k}$ is given by

$$
k=K-K^{\prime} .
$$

Thus, if for a given real lattice we can enumerate $S_{n}$ and $M_{n}$ for sufficiently large $n$, then we can calculate $k$ for the T-CT which, as we have argued above, corresponds to the real lattice, so far as the one-to-one correspondence between the branches of the т-ст and the closed saws in the real lattice is concerned. For a given real lattice, this is the $k$ we should use in the exact localisation treatment of AAT and obtain almost exact localisation results for the real lattice.

We have calculated $k$ for three two-dimensional lattices, namely, triangular, square and honeycomb using the $S_{n}, M_{n}$ data provided by P Grassberger. Table 1 lists $S_{n}$, $M_{n}^{i}$ (number of walks with $i$ possibilities for the next step) and

$$
M_{n}\left(=\sum_{i=1}^{K-1} M_{n}^{i}\right)
$$

for the square lattice. The values given are only for a few short walks to help the reader understand the definitions of $S_{n}$ and $M_{n}$. The $S_{n}$ and $M_{n}$ were enumerated for sufficiently long walks. The maximum number of steps was $n=30$ for the honeycomb, $n=18$ for the square and $n=15$ for the triangular lattice for which $S_{n} / C$ was extremely large62166075,31164683 and 963627597 , respectively. These numbers are high enough for very good statistics, e.g., the variation in $S_{n} / M_{n}$, the quantity of interest in equation (6), becomes smooth with respect to $n$ well before the highest value of $n$ given above. This enabled us to extrapolate easily the asymptotic value of $S_{n} / M_{n}$ for $n \rightarrow \infty$. The values of $K, K$ and $k$ are compared for these lattices in table 2.

Table 1. For a square lattice ( $C=4 ; K=3$ ) are listed a sample of values of total number of sAWs of $n$ steps as well as the groups of these SAws that after the $n$th step have $i$ possibilities available for taking the next step. The numbers pertain to only one of the four directions from the origin, so the $S_{n}, M_{n}^{i}$ and $M_{n}$ will be four times the above numbers. Note that $S_{n}=\Sigma_{i=1}^{K} M_{n}^{i}$, where $i$ is the connectivity on $M_{n}^{i}$ points $n$ steps away from the origin. For actual calculations of $S_{n} / M_{n}$, these numbers were calculated for $n$ up to 18,15 and 30 for square, triangular and honeycomb lattices, respectively.

|  | $M_{n}^{i} / C$ |  |  |  |  |  |
| :--- | ---: | :--- | :--- | ---: | ---: | :--- |
| $n$ | $S_{n} / C$ | $i=0$ | $i=1$ | $i=2$ | $i=3$ | $M_{n} / C=\sum_{i=1}^{K-1} M_{n}^{i} / C$ |
| 2 | 3 | 0 | 0 | 0 | 3 | 0 |
| 3 | 9 | 0 | 0 | 2 | 7 | 2 |
| 4 | 25 | 0 | 0 | 4 | 21 | 4 |
| 5 | 71 | 0 | 2 | 14 | 55 | 16 |
| 6 | 195 | 0 | 4 | 34 | 157 | 38 |
| 7 | 543 | 2 | 18 | 108 | 415 | 128 |
| 8 | 1479 | 4 | 42 | 274 | 1159 | 320 |

Table 2. Comparison of the connectivity constant $k$ for a trimmed Cayley tree corresponding to three two-dimensional lattices, with the conventional connectivity constant $\boldsymbol{K}$ associated with these lattices (obtained by counting the saws), and $K$ which is simply $C-1$ ( $C \equiv$ coordination number).

| Lattice type | $\boldsymbol{k}^{\mathrm{a}}$ | $\boldsymbol{K}^{\mathrm{b}}$ | $\boldsymbol{K}$ | $\boldsymbol{C}$ |
| :--- | :--- | :--- | :--- | :--- |
| Honeycomb | 1.191 | 1.848 | 2 | 3 |
| Square | 1.354 | 2.639 | 3 | 4 |
| Triangular | 1.689 | 4.151 | 5 | 6 |

${ }^{\text {a }}$ Equation (6'); the maximum value of $n$ was 30 for the honeycomb, 18 for the square and 15 for the triangular lattice.
${ }^{\text {b }}$ Equation (4).

We used Newton's 'divided-difference' method (see, e.g., Zurmühl 1976) to do a stepwise extrapolation. For example, for a triangular lattice first we fitted the following fifth-order polynomial over the six $S_{n} / M_{n}$ points corresponding to $n=10-15$ :
$f(n)=a_{0}+(n-10) a_{1}+(n-10)(n-11) a_{2}+\ldots+(n-10)(n-11) \ldots(n-14) a_{5}$
then calculated $f(16)$ from this and used this new point to enlarge the polynomial to sixth order, then calculated $f(17)$ from this and enlarged the polynomial to seventh order, and so on. The advantage of this method is that each time a new point becomes available to enlarge the polynomial, only one extra coefficient, say $a_{i}$, needs to be calculated leaving all previous ( $a_{0}, \ldots, a_{i-1}$ ) coefficients unchanged. This process was continued until two successive values of $S_{n} / M_{n}$ became very close to each other. Even after that we took a conservative estimate for the asymptotic value of $S_{n} / M_{n}$ (see figure 3) to avoid the possibility of the above extrapolation procedure overestimating it. However, we may add that there is hardly a scope for the latter to happen because the error in the divided-difference method is known to decrease rapidly as the order of the polynomial increases. In the present case it becomes infinitesimal for $f(n)$ of the order of five or so.


Figure 3. $S_{n} / M_{n}$ versus $n$ for the triangular lattice. The crosses represent the points obtained by a stepwise extrapolation. The curve has been drawn to guide the eye.

We mention in passing the following interesting identity observed by us,

$$
\begin{align*}
\lim _{n \rightarrow 0}\left(\frac{S_{n+1}}{S_{n}}=\right. & \frac{M_{n+1}}{M_{n}}=\frac{S_{n+1}-M_{n+1}}{S_{n}-M_{n}}=\frac{B_{n+1}}{B_{n}}=\frac{M_{n+1}^{0}}{M_{n}^{0}} \\
& \left.=\frac{M_{n+1}^{1}}{M_{n}^{1}}=\frac{M_{n+1}^{2}}{M_{n}^{2}}=\ldots=\frac{M_{n+1}^{K-1}}{M_{n}^{K-1}}\right)=K=(K-1)^{\lambda} \tag{7}
\end{align*}
$$

where $B_{n}$ represents the number of blocked steps at the stage $n$ and the $M_{n}^{i}$ represent the number of sites with $i$ possibilities to step further; $\lambda$ is an exponent that depends on the lattice dimensionality only (Srivastava 1984).

## 5. Localisation in the т.cт

We have understood that the convergence of the RPS (1 or 2 ) is predominantly governed by the two-step saws $V_{i j} V_{j i}, V_{j k} V_{k j}, \ldots$, that appear in the respective first terms of the RPSs for $S_{i}, S_{i}^{i}, S_{k}^{i, j}$, etc. If we ignore all the higher terms and retain only the first one in $S_{i}, S_{j}^{i}$, etc., and if for each this term consists of $K$ steps (corresponding to the $K=C-1$ neighbours in the 'forward' direction), then a continued fraction consisting of $S_{i}, S_{j}^{i}$ etc., will represent a ct of connectivity $K$. However, as we have seen in previous sections, if we look at a SAW performed on a real lattice then at an arbitrary stage $m$ the number of steps, $V_{m n} V_{n m}$, is constrained by the requirement that $n \neq i, j, \ldots m$ where $i, j, k, \ldots$, are the sites covered by the saw before reaching site $m$. The number of steps from $m$ can be anywhere between 0 and $K$. Further, we have seen that it is not the number of steps taken from the site $m$ that interest us, but rather it is the number of blocked steps, which can not be taken from $m$. A t-ct consisting of such branches is the one that we will use for the localisation studies of the real lattice under consideration.

The continued fraction representing this t-CT has been found by Srivastava and Chaturvedi (1982) by rewriting the whole (convergent) RPS in the form of a single
continued fraction with the contribution of each SAW in the hierarchy properly fed into the denominators of the continued fraction of the first term. The continued fraction derived there was the representation for the T-CT constructed here. The study of the convergence properties of this continued fraction showed that the convergence of the RPS $\Leftrightarrow$ the convergence of the 'renormalised' continued fraction (representing the T-CT). Thus, an eigenstate having a localised wavefunction on the T-CT will also be localised in the real lattice. The nature of distribution of eigenenergies in the tree lattices is quite different from that of the real lattices; in particular, the former have smaller band widths. So a localised state in a real lattice will correspond either to a localised state in the corresponding т-CT or to an energy outside the T-CT band states. In any case, the mobility edge $E_{\mathrm{c}}$ will appear at the same energy in both the lattices if the energy scales of the two are taken to be the same with the zeros coincidental.

Since the density of states in a real lattice and that in the corresponding т-ст are different, the calculation of the localisation length will yield different results for the two. In fact, due to the non-intersecting branches in a ct the shape of a wavefunction spread over it is very different from that in a real lattice-it has a highly ramified octopuslike shape and the localisation length is a measure of the distance penetrated by the wavefunction along a branch. However, since $E_{c}$ occurs at the same energy in the two, the $E_{\mathrm{c}}$ versus $W$ trajectories and the $W_{\mathrm{c}}$ are the same for the two lattices.

Thus, after $\boldsymbol{k}$ has been calculated from relation ( $6^{\prime}$ ) for a T-Ст corresponding to a given real lattice (represented in ( $6^{\prime}$ ) by $K=C-1, K, S_{n}$ and $M_{n}$ ), all we need to do is to use the exact formulation of AAT (1973) and Abou-Chacra and Thouless (1974) to solve the localisation problem; for instance, obtain $W_{\mathrm{c}}$ from condition (3) and $E_{\mathrm{c}}-W$ trajectories from the relations given in AAT (§7) for different types of distributions for site energies $e_{i}$. These results will be the nearly exact results for the real lattice. As an example we compute $W_{c}$ for the two-dimensional lattices for which we have calculated $\boldsymbol{k}$.

## 6. Ambiguity of two dimensions

We have chosen two-dimensional lattices for our computations because (a) $S_{n}$ and $M_{n}$ can be enumerated for larger values of $n$ than for the three-dimensional lattices, and ( $b$ ) two-dimensional systems are of particular interest in view of the prediction of Abrahams et al (1979) that complete localisation will occur even at infinitesimal disorder. Our results are quite interesting with an element of surprise as discussed below.

The critical value of disorder $W_{c}$ at which the Anderson transition takes place (i.e., when the whole band consists of localised eigenstates) is given for a rectangular distribution of random site energies, from (3) as,

$$
W_{\mathrm{c}}=4 K V \ln \left(W_{\mathrm{c}} / 2 V\right)
$$

As stated earlier this result comes from Anderson's (1958) theory for a real lattice of connectivity $K$ as well as from the exact treatment of aAT (1973) for a CT of connectivity $K$. Having argued that for the calculation of $W_{\mathrm{c}}$ and $W_{\mathrm{c}}-E$ trajectories we can treat a T-CT of connectivity $\boldsymbol{k}$ as exactly equivalent to a real lattice of connectivity $\boldsymbol{K}$ (or coordination number $C$ ), we can respectively use ( $3^{\prime}$ ) for the band centre, and $W_{c}=$ $2 K V \ln \left[\left(W_{\mathrm{c}}^{2} / 4-E^{2}\right) / V^{2}\right]$ for other values of $E$ [the same as equation (7.8) of aAT (1973)] to obtain the exact results for a real lattice. We solved ( $3^{\prime}$ ) for a series of values


Figure 4. $W_{c}$ versus $K$ obtained by solving equation ( $3^{\prime}$ ) for the band centre and for a series of $C T$ connectivity $K$ values. The solutions shown by the bold line are the relevant ones. The arrows $\uparrow$ on the $K$ axis indicate $k$ values for the two-dimensional lattices studied. The dots on the bold line denote values of $W_{c}$ for honeycomb ( HC ) and square ( sQ ) lattices with $K=$ 2 and 3 , respectively; the value corresponding to the triangular ( TR ) lattice is outside the range of the diagram. The cross shows the value of $W_{c}$ for a triangular lattice corresponding to $k$.
of $K$ and the results are shown in figure 4 . For each $K$ there are two solutions for $W_{c}$, but only the larger solution is of interest ( D J Thouless, private communication). At $K \equiv K_{\mathrm{c}}=1.36$ both solutions merge and no solution exists for $K<K_{\mathrm{c}}$. The meaning of the non-existence of a solution for $K<K_{\mathrm{c}}$ is, according to AAT, that the localised state at the band centre is always stable even for infinitesimal $W$. Therefore, for a real lattice if the value of $k$ falls below $K_{\mathrm{c}}$ all states will be localised for any amount of disorder. We find that for the honeycomb lattice $k(=1.19)$ is clearly below $K_{\mathrm{c}}$, for the square lattice $\boldsymbol{k}(=1.35)$ is very close to $K_{c}$, and for the triangular lattice $k(=1.69)$ is sufficiently above $K_{c}$. This implies that the Abrahams et al (1979) contention holds for the honeycomb and the square lattices with the square lattice being the marginal case; however, the triangular lattice does have the mobility edges.

The case of square lattice is particularly interesting and requires special mention because there are several estimates of $W_{\mathrm{c}}$ available for it. The value of $W_{\mathrm{c}} / V$ (with $V=$ 1) expected from the present calculation (from figure 4) is very close to 6 , which should be compared with the previous numerical and analytical estimates listed below:

Numerical estimate of Licciardello and Thouless (1975) 6.1

Numerical estimate of Weaire and Srivastava (1977) 6.0
Numerical estimate of Stein and Krey (1980) 6.5
Analytical estimate of Anderson (1958)
Analytical estimate of Economou and Cohen (1972)
Analytical estimate of Abou-Chacra et al (1974)
Analytical estimate of Licciardello and Economou (1975)
Analytical estimate of Brouers and Kumar (1975)
Clearly, the agreement of the numerical estimates, all obtained by different methods, with present estimates is excellent. Similarly, the previous numerical estimates for triangular lattice, were (approximately) 9.4 by Licciardello and Thouless (1975), and
$9.5( \pm 0.5)$ by Stein and Krey (1981), which agree well with the present value of 11.5 (from figure 4). It is hard to judge whether this agreement is coincidental or real. If real, it lends strong support to the numerical estimates which are otherwise taken with scepticism, especially the results on two-dimensional systems after the Abrahams et al (1979) conjecture.

Note that it is generally believed that there should exist in the localisation problem a marginal dimension at and below which the disordered system should behave like an insulator and no metal-insulator transition should occur. That a marginal connectivity constant can exist is surprising. This surprising result should be understood and appreciated in light of the fact that it was obtained from the exact theory worked out for tightbinding Hamiltonians, i.e., in the strong disorder limit ( $W \gg V$ ). The subtle weak localisation effects (Bergmann 1984), therefore, can not play a role here. Consequently, if the triangular lattice has mobility edges and requires rather high critical disorder to merge them into one (the Anderson transition), it seems unlikely that an alternative approach worked out in the weak disorder limit should yield more localisation than has been found here. Besides working in the strong disorder limit, since we obtain our result by mapping the real lattice onto a т-ст in which, by the very nature of its geometry, the localisation is difficult, and since our mapping is exact, we believe that the localisation in real lattices is more difficult than generally believed following the result of Abrahams et al (1979). Indeed, the localisation is not as difficult as indicated in the original results of Anderson (1958) and AAT (1973). The reasons for the small difference between our result and that of Abrahams et al (1979) may be the subtle effects discussed by Phillips (1983) and the fact that the single-parameter theory of Abrahams et al (1979) is not good enough for localisation studies (see, e.g., Ioffe et al 1985).

## 7. Conclusion

We conclude that the old theories of Anderson (1958) and AAT (1973) are still the most rigorous ones available for localisation studies. In particular, the self-consistent theory of AAT which is exact for the Cayley tree lattice and hitherto believed to give highly approximate results for real lattices has been shown here to be extremely good for studying localisation in real lattices provided care is taken in isolating those branches in the CT that are relevant for a particular real lattice. This is done by mapping the saws on a real lattice that contribute to the RPS ( 1 or 2 ) onto the CT and then trimming off unwanted branches. The connectivity constant for a T-CT obtained in this fashion can be calculated exactly, and when this is substituted in the AAT theory estimates of the critical disorder $W_{\mathrm{c}}$ and the mobility edge trajectories, etc., can be calculated for the real lattice. Calculations for two-dimensional lattices reveal the surprising result that the honeycomb lattice never has mobility edges, whereas the triangular lattice does seem to have them, and the square lattice is a borderline case.

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## References

Abou-Chacra R, Anderson P W and Thouless D J 1973 J. Phys. C: Solid State Phys. 61734-52
Abou-Chacra R and Thouless D J 1974 J. Phys. C: Solid State Phys, $765-75$
Abrahams E, Anderson P W, Liciardello D C and Ramakrishnan T V 1979 Phys. Rev. Lett. 42 673-6
Anderson P.W 1958 Phys. Rev. 109 1492-505
Bergmann G 1984 Phys. Rep. 107 1-58
Brouers F and Kumar N 1975 Solid State Commun. 17 1453-7
Economou E N and Cohen M H 1972 Phys. Rev. B 5 2931-48
Elyutin P V, Hickey B, Morgan G J and Weir G F 1984 Phys. Stat. Solidi (b) 124 279-85
Ioffe L B, Sagdeev I R and Vinokur V 1985 J. Phys. C: Solid State Phys. 18 L641-6
Lee P A and Ramakrishnan T V 1985 Rev. Mod. Phys. 57 289-337
Licciardello D C and Economou E N 1975 Phys. Rev. B $113697-717$
Licciardello D C and Thouless D J 1975 J. Phys. C: Solid State Phys. $84157-70$
-_ 1978 J. Phys. C: Solid State Phys. $11925-36$
Mott N F and Davis E A 1979 Electronic Processes in Non-Crystalline materials (Oxford: Clarendon)
Phillips J C 1983 Solid State Commun. 47 191-3
Schreiber M 1987 J. Non-Cryst. Solids 97/98 221-24
Srivastava V 1984 Z. Physik B 56 161-3
Srivastava V and Chaturvedi M 1982 J. Phys. C: Solid State Phys. 15 L215-20
Stein J and Krey U 1980 Z. Physik B 37 13-22
-_ 1981 Physica A 106 326-43
Thouless D J 1970 J. Phys. C: Solid State Phys. 3 1559-66
Weaire D and Srivastava V 1977 J. Phys. C: Solid State Phys. 21 4309-18
Zurmühl R 1976 Numerical Analysis for Engineers and Physicists (Berlin: Springer)


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