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## Evaluation of the Kubo formula for conductivity using the recursion method

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**Abstract.** We propose a numerical algorithm based on the recursion method to calculate the conductivity of a disordered system described by a tight-binding Hamiltonian. It has the advantage that the density of states and the conductivity can be obtained in a single recursion calculation. The method is applied to simple one- and two-dimensional incommensurate systems in order to check the validity of the assumptions made and the numerical efficiency. The calculated conductivity shows a clear drop when the Fermi energy crosses a mobility edge. Potential applications of this work to other systems are discussed.

### 1. Introduction

There are two general approaches to calculating transport properties in disordered materials.

(i) In quasi-one-dimensional (1D) systems the transfer matrix technique [1] can be used to calculate the transmission or reflection coefficients, which are associated with the conductance by Landauer's formula [2]. This type of approach has been used in [3] for wires of different cross sections to study the Anderson transition in three dimensions as a limiting case.

(ii) The conductivity can be calculated using the Kubo–Greenwood formula, derived as a special case of the fluctuation–dissipation theorem [4]. It has been generally treated in a mean-field approximation because direct calculations require an enormous amount of computing time, even for moderate-size systems [5]. However, the mean field approaches either neglect [6] or estimate roughly [7] the vertex part of the conductivity, destroying the quantum interference that gives rise to localisation in disordered systems.

In this paper we devise a formalism based on the recursion method in [8] to evaluate the Kubo–Greenwood formula. It avoids the shortcomings of the mean-field approximations and is very efficient from the numerical point of view.

The recursion method is usually used for the calculation of the electronic local densities of states. Starting from a local orbital, it constructs a new basis in which the Hamiltonian is tridiagonal. However, for the conductivity there is another relevant operator apart from the Hamiltonian, namely the momentum operator.

In previous work [9] it was shown that a generalised matrix form of Dyson's equation may be written which relates a product of Green functions that essentially gives the conductivity with the momentum operator and the Hamiltonian. Although it is in general not possible to tridiagonalise simultaneously the Hamiltonian and the momentum operator, we show in this work that the use of the basis obtained by the usual recursion method, with a conveniently chosen starting orbital, allows the calculation of both the density of states and the conductivity in a single recursion algorithm. However, one should note that the effects of truncation of the recursion basis set are different for each property and must be studied separately.

A different idea, also based on the recursion method, was proposed in [10] to calculate the conductivity of disordered two-dimensional (2D) and three-dimensional (3D) systems. The recursion method was used to obtain approximate eigenstates of the Hamiltonian, which allowed the matrix elements of the Green functions and the momentum operator in the Kubo formula to be evaluated. Our approach is different as it does not require knowledge of the eigenvectors but only the recursion basis set. We believe that our presentation of the problem in a matrix form plus the adequate choice of the starting vector make a simpler numerical solution possible, more in the spirit of the original recursion method [8].

This paper is organised as follows. In § 2 we first write the Kubo–Greenwood formula in a notation that is convenient for calculation in a tight-binding scheme. We then show that a continued-fraction expansion for the conductivity of a 1D system is possible and then we introduce our approximation that uses the recursion method for the general case (more than one dimension). Section 3 contains the numerical examples used to test the method. We started with a 1D incommensurate system, well known to us from previous work [11], that shows an abrupt change in the localisation length (possibly a mobility edge). As a second step, we studied a 2D model that also shows a mobility edge. The model was constructed in such a way that its density of states and conductivity could be obtained from the corresponding properties of the previous 1D example and therefore was useful to check the present method.

## 2. Calculation of the conductivity

### 2.1. The Kubo formula in a convenient tight-binding notation

The DC electrical conductivity in the linear response approximation is given by the Kubo–Greenwood formula. At zero temperature and for non-interacting electrons, it can be written in terms of Green functions as [6]

$$\sigma_{xx}(E) = (K/\Omega) \text{Tr}\{p_x \text{Im}[G^+(E)]p_x \text{Im}[G^+(E)]\} \quad (1)$$

where  $K$  is a universal constant,  $\Omega$  is the system volume,  $E$  is the Fermi energy and the Green functions are defined by  $G(z) = (z - H)^{-1}$  and

$$G^\pm(E) = \lim_{\eta \rightarrow 0} [G(E \pm i\eta)].$$

We consider the Hamiltonian defined in the site representation as

$$H = \sum_i \varepsilon_i |i\rangle\langle i| + \sum_{i \neq j} V_{ij} |i\rangle\langle j| \quad (2)$$

and assume interactions only between first neighbours with a fixed value  $V$ . This is taken

as unit of energy. The diagonal element  $\varepsilon_i$  is a variable assumed to be distributed according to a different law for each non-periodic problem.

For simplicity, we shall consider only simple cubic 1D, 2D or 3D lattices and take the lattice parameter as unit of length. The momentum operator  $p_x$  can be replaced in (1) by the commutator  $C_x = [H, x]$  (which is real in the site representation) with the proper redefinition of the constant  $K$ . If  $j + 1$  indicates the first neighbour of site  $j$  in the positive  $x$  direction, the operator  $C_x$  may be expressed as

$$C_x = \sum_j (|j\rangle\langle j + 1| - |j + 1\rangle\langle j|). \tag{3}$$

It is convenient to define new operators for the calculation of  $\sigma_{xx}(E)$ . If  $S^\pm(E) = G^\pm(E)C_xG^\pm(E)$ , then

$$S^+(E) - S^-(E) = 2iG^+(E)C_x \text{Im}[G^+(E)] \tag{4}$$

and

$$\text{Re}[S^+(E) - S^-(E)] = -2 \text{Im}[G^+(E)C_x \text{Im}[G^+(E)]]. \tag{5}$$

Replacing (5) in (1), we obtain

$$\sigma_{xx}(E) = (K/\Omega) \text{Tr}\{C_x \text{Re}[S^+(E) - S^-(E)]\} \tag{6}$$

and, using (3),

$$\sigma_{xx}(E) = \frac{K}{2\Omega} \sum_j \{[S_{jj+1}^+(E) - S_{j+1j}^+(E)] + [S_{jj+1}^-(E) - S_{j+1j}^-(E)]\}. \tag{7}$$

This expression is suitable for the evaluation of the conductivity in the site representation.

### 2.2. Recursion equations for one-dimensional systems

It can be shown [9] that  $G^\pm$  and  $S^\pm$  satisfy a set of coupled integral equations. If we decompose  $H = h + V$ , where  $h$  is the diagonal part of the Hamiltonian and the corresponding Green function is  $g(z) = (z - h)^{-1}$ , then

$$G^\pm = g^\pm(1 + VG^\pm) \tag{8}$$

and, replacing this in the definition of  $S^\pm$ ,

$$S^\pm = g^\pm(C_x G^\pm + VS^\pm). \tag{9}$$

These two expressions can be formally put together in a single matrix equation

$$\mathbf{G}^\pm = \mathbf{g}^\pm(\mathbf{1} + \mathbf{V}\mathbf{G}^\pm) \tag{10}$$

where the generalised operators  $\mathbf{G}^\pm$ ,  $\mathbf{g}^\pm$  and  $\mathbf{V}$  are given by

$$\mathbf{G}^\pm = \begin{pmatrix} G^\pm & 0 \\ S^\pm & G^\pm \end{pmatrix} \quad \mathbf{g}^\pm = \begin{pmatrix} g^\pm & 0 \\ 0 & g^\pm \end{pmatrix} \quad \mathbf{V} = \begin{pmatrix} V & 0 \\ C_x & V \end{pmatrix}.$$

Note that each matrix element of a generalised operator is itself a  $2 \times 2$  matrix, e.g.

$$\mathbf{G}_{ij}^\pm = \begin{pmatrix} G_{ij}^\pm & 0 \\ S_{ij}^\pm & G_{ij}^\pm \end{pmatrix}.$$

Because of the similarity of equation (10) to Dyson's equation, all real-space methods

used to calculate the density of states of disordered systems could be applied to obtain simultaneously, and within the same approximation, the density of states and the conductivity. For example, by direct analogy with the recursion method formalism, one can expand  $\mathbf{G}_{00}$  as a continued fraction for the case of a semi-infinite chain (here the subscript 0 denotes the first site of the chain). This is so because in this particular example both  $V$  and  $C_x$  are tridiagonal in the site representation. The continued-fraction expansion will be given by

$$\mathbf{G}_{00} = \{ \mathbf{1} - \mathbf{g}_0 \mathbf{V}_{01} [ \mathbf{1} - \mathbf{g}_1 \mathbf{V}_{12} ( \mathbf{1} - \dots )^{-1} \mathbf{g}_2 \mathbf{V}_{21} ]^{-1} \mathbf{g}_1 \mathbf{V}_{10} \}^{-1} \mathbf{g}_0 \quad (11)$$

where

$$g_l(z) = (z - \varepsilon_l)^{-1} \quad \mathbf{V}_{l+1} = \begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix} \quad \mathbf{V}_{l+l} = \begin{pmatrix} 1 & 0 \\ -1 & 1 \end{pmatrix}.$$

To evaluate the conductivity of an infinite linear chain using (7) we need the off-diagonal elements  $S_{jj+1}^{\pm}$ , that are included in  $\mathbf{G}_{jj+1}^{\pm}$ . These can be obtained by matching two continued fractions such as (11): one corresponding to the semi-infinite chain to the left of  $j$  ( $\mathbf{G}_{jj}^L$ ) and the other corresponding to the semi-infinite chain from  $j+1$  to the right ( $\mathbf{G}_{j+1j+1}^R$ ). It is easy to show that the desired quantity is given by

$$\mathbf{G}_{jj+1} = [ \mathbf{1} - \mathbf{G}_{jj}^L \mathbf{V}_{jj+1} \mathbf{G}_{j+1j+1}^R \mathbf{V}_{j+1j} ]^{-1} \mathbf{G}_{jj}^L \mathbf{V}_{jj+1} \mathbf{G}_{j+1j+1}^R. \quad (12)$$

In the calculations that use the present formalism, the time required to evaluate the conductivity of a linear chain increases linearly with increase in the number of sites considered. In this sense it is equivalent to the algorithm proposed in [12].

### 2.3. Use of the recursion method in the general case

In more than one dimension it is not possible to find a basis where both  $V$  and  $C_x$  adopt a tridiagonal form. If we use the recursion method to obtain a basis that tridiagonalises  $H$ , then  $C_x$  will in principle connect all the elements of this new basis. However, we can use the recursion basis set to evaluate the elements of  $S_{jj+1}^{\pm}$  in a way that is less time consuming than the calculation of all the matrix elements of  $G$  in the site representation (as was done in [5] for a Penrose lattice).

Given a starting orbital  $|v_0\rangle$ , the equations which define the recursion method are

$$\begin{aligned} b_0 |v_1\rangle &= H|v_0\rangle - a_0 |v_0\rangle \\ b_1 |v_2\rangle &= H|v_1\rangle - a_1 |v_1\rangle - b_0^* |v_0\rangle \\ b_n |v_{n+1}\rangle &= H|v_n\rangle - a_n |v_n\rangle - b_{n-1}^* |v_{n-1}\rangle \end{aligned} \quad (13)$$

where the coefficients  $a_n, b_n$  are obtained imposing the orthonormalisation condition  $\langle v_m | v_n \rangle = \delta_{mn}$ . The diagonal element of the Green function  $\langle v_0 | G | v_0 \rangle$  is then given by a continued fraction

$$\begin{aligned} \langle v_0 | G(z) | v_0 \rangle &= [z - a_0 - |b_0|^2 \Delta_1(z)]^{-1} \\ \Delta_1(z) &= [z - a_1 - |b_1|^2 \Delta_2(z)]^{-1} \\ \Delta_n(z) &= [z - a_n - |b_n|^2 \Delta_{n+1}(z)]^{-1}. \end{aligned} \quad (14)$$

As the system Hamiltonian in the recursion basis is equivalent to that of a semi-infinite

chain, it is also possible to obtain the matrix elements  $\langle v_0 | G | v_n \rangle$  by replacement in the truncated set of coupled equations obtained from equation (8):

$$\langle v_0 | G | v_n \rangle = \langle v_0 | G | v_0 \rangle \prod_{l=0}^n b_l^* \Delta_{l+1}. \quad (15)$$

If after each recursion step the components of the states  $|v_n\rangle$  in site representation are stored, then the elements of  $C_x$  in the new basis can also be calculated using equation (3). Therefore,  $\langle v_0 | S | v_0 \rangle$  can be obtained in a single recursion calculation by

$$\langle v_0 | S | v_0 \rangle = \sum_{nm} \langle v_0 | G | v_n \rangle \langle v_n | C_x | v_m \rangle \langle v_m | G | v_0 \rangle. \quad (16)$$

The first step is to note which starting orbitals are useful for the conductivity calculation. If

$$|v_{0j}^{\pm}\rangle = (1/\sqrt{2})(|j\rangle \pm i|j+1\rangle) \quad (17)$$

then

$$\langle v_{0j}^+ | S | v_{0j}^+ \rangle - \langle v_{0j}^- | S | v_{0j}^- \rangle = i(S_{jj+1} - S_{j+1j}) \quad (18)$$

which gives the quantity required in equation (7). There are also some properties satisfied by the matrix elements of  $G$  and  $C_x$  that simplify the calculation. The coefficients  $b_n$  are determined from the recursion equations (13) except for an arbitrary phase, which can be chosen equal to zero [13]. It can be shown that this choice implies

$$\begin{aligned} \langle v_n^+ | C_x | v_m^+ \rangle &= \langle v_n^- | C_x | v_m^- \rangle^* \\ \langle v_0^+ | G | v_n^+ \rangle &= \langle v_0^- | G | v_n^- \rangle \end{aligned} \quad (19)$$

where we have omitted the subscript  $j$  in  $|v_{nj}\rangle$  and shall continue to do so for simplicity. It is then sufficient to work with only one starting orbital  $|v_0^+\rangle$ . When equations (7), (18) and (19) are taken into account, the conductivity will be given by

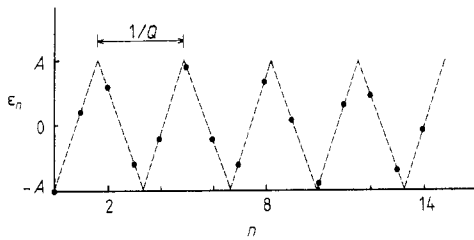
$$\sigma_{xx}(E) = \frac{K}{\Omega} \sum_j [S_j^+(E) - S_j^-(E)] \quad (20)$$

with

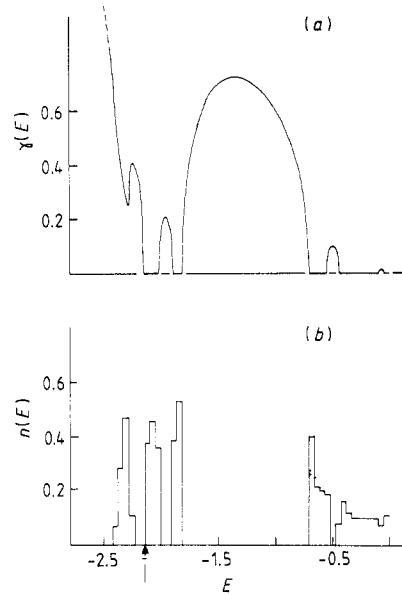
$$S_j^{\pm}(E) = \sum_{mn} \langle v_0 | G^+ | v_n \rangle \text{Im}[\langle v_n | C_x | v_m \rangle] \langle v_m | G^{\pm} | v_0 \rangle.$$

The exact result for an infinite system is obtained when the number  $N$  of steps in the recursion tends to infinity and the imaginary part of the energy  $\eta$  tends to zero. However, in a numerical calculation,  $\eta$  must be larger than  $N^{-1}$  in order to eliminate statistical fluctuations due to the discreteness of the number of states. This is equivalent to the effect of an inelastic mean free path, beyond which localisation effects cannot be detected.

Another approximation of any numerical work in a non-periodic system is to replace the trace operation in (7) by an average over a set of randomly selected sites. The number of sites that give representative results will be discussed in § 3 in relation to the examples. Also, we show that it is possible to simplify further the computation by neglecting the elements  $\langle v_n | C_x | v_m \rangle$  when  $|n - m|$  becomes sufficiently large. This is a consequence of the nature of the recursion basis states that spread out from the starting sites.



**Figure 1.** Site self-energies on a linear chain with an incommensurate zigzag modulation. The amplitude  $A$  and wavevector  $Q$  of the modulation are defined in the figure.



**Figure 2.** (a) The exponential growth factor  $\gamma(E)$  of the wavefunctions and (b) the density  $n(E)$  of states for the system in figure 1 with  $A = 1.5$ . Only half of the band is shown.

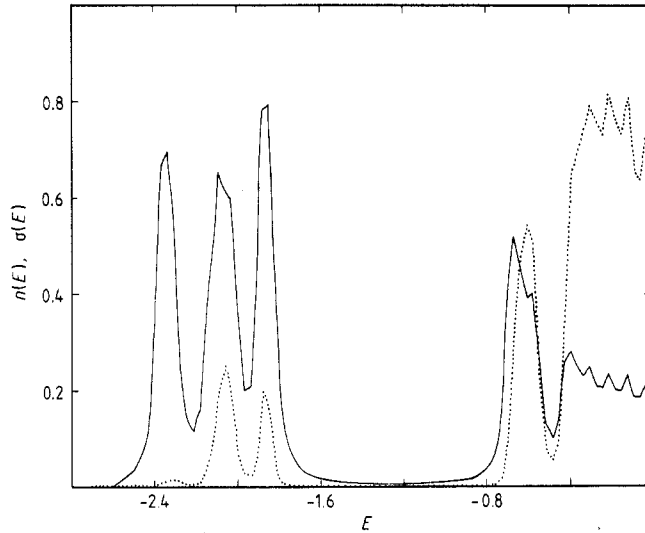
### 3. Numerical examples

#### 3.1. One-dimensional incommensurate system

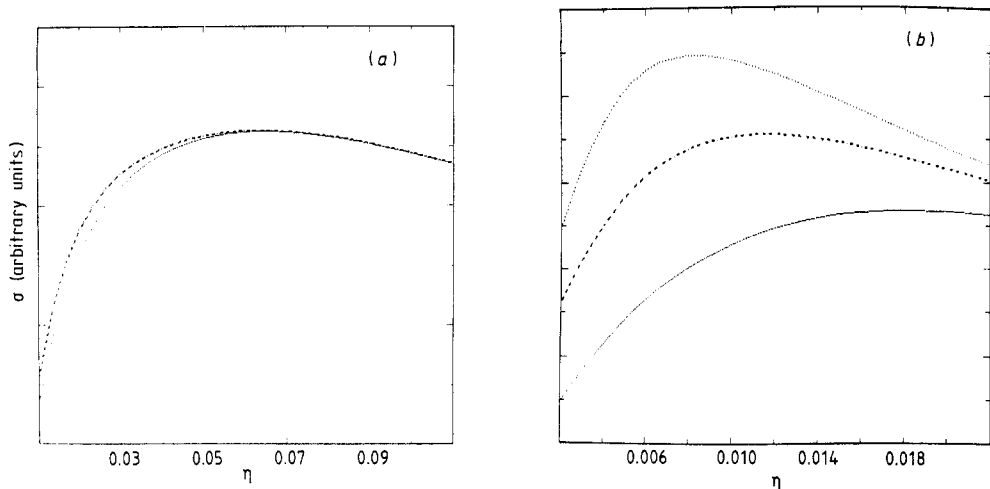
Previous work on 1D incommensurate systems shows that they may have mobility edges in certain cases. In particular, the localisation of the wavefunctions in the case of a zigzag modulation of the site energies was studied by Llois and co-workers in [11] by the transfer matrix technique. They found a metal–insulator transition when the amplitude of the modulation approximately exceeded the half-band width.

We have chosen one of their examples, with a well defined mobility edge, to test our present method. The zigzag modulation is shown in figure 1, and in figure 2 we reproduce the results of [11] for the density  $n(E)$  of states and the exponential growth factor  $\gamma(E)$ , which is the inverse of the localisation length. Only the states in the lower sub-band are localised, and we expect to see this reflected by zero conductivity in our calculations.

In figure 3 we show the results for  $n(E)$  and  $\sigma(E)$  obtained using  $N = 50$ ,  $\eta = 0.025$  and averaging over 20 sites. As can be seen by comparing figures 2 and 3 this level of approximation is sufficient to obtain the main structure of the density of states. The conductivity is also in agreement with what could be expected from the character of the wavefunctions. However, further insight can be gained by studying the behaviour of  $\sigma(E, \eta)$  as a function of  $N$ . Figure 4 shows  $\sigma(\eta)$  for two values of the energy  $E$  and several values of  $N$ . For  $E = -2.15$ , an energy below the mobility edge, the curves are almost independent of  $N$  even for the small values of  $N$  considered. This proves that the states are localised within the scales considered. In contrast, for  $E = -2.05$  there is always a maximum of  $\sigma$  as a function of  $\eta$  that moves towards  $\eta = 0$  and increases in height



**Figure 3.** Density of states (—) and conductivity (⋯) for the same system as in figure 2, calculated with the recursion equations described in § 2.2. The conductivity is given in arbitrary units.



**Figure 4.** Conductivity as a function of  $N$  and  $\eta$  for (a)  $E = -2.15$  and (b)  $E = -2.1$ : —,  $N = 20$ ; ----,  $N = 30$ ; ⋯,  $N = 50$ .

linearly with increasing  $N$ . In this region of extended states, the conductivity seems to diverge with increasing  $N$  in the same way as in a periodic system.

Another example with a larger modulation amplitude is shown in figure 5. The mobility edge in this case is closer to the centre of the band ( $E = -1.8$ ).

### 3.2. A two-dimensional incommensurate example

It is possible to construct a 2D system whose solution for both  $n(E)$  and  $\sigma(E)$  can be obtained from the known results of a 1D system.



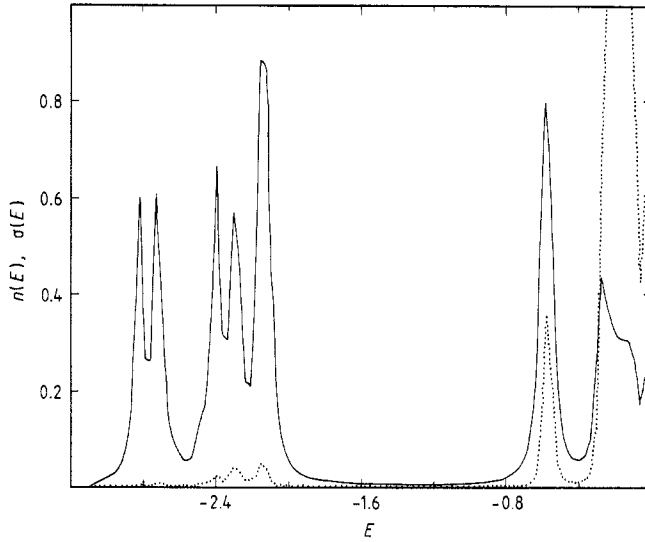


Figure 5. Same as figure 3 for a larger modulation amplitude  $A = 2.2$ .

Let us consider a square lattice and indicate by  $|ij\rangle$  the basis orbital at site with coordinates  $x = i$  and  $y = j$ . If the Hamiltonian can be decomposed as  $H = H_x + H_y$ , where  $H_x$  does not act on the  $y$  coordinate and  $H_y$  does not act on the  $x$  coordinate, then it is easy to prove that the eigenstates are a direct product of two eigenstates of a 1D problem.

For example, we can take the site energy on site  $(i, j)$  as  $\varepsilon_i + \varepsilon_j$ , where  $\varepsilon_i$  and  $\varepsilon_j$  are the site energies of the 1D incommensurate system already studied. In this case the density of states and the conductivity of the 2D system will be given by

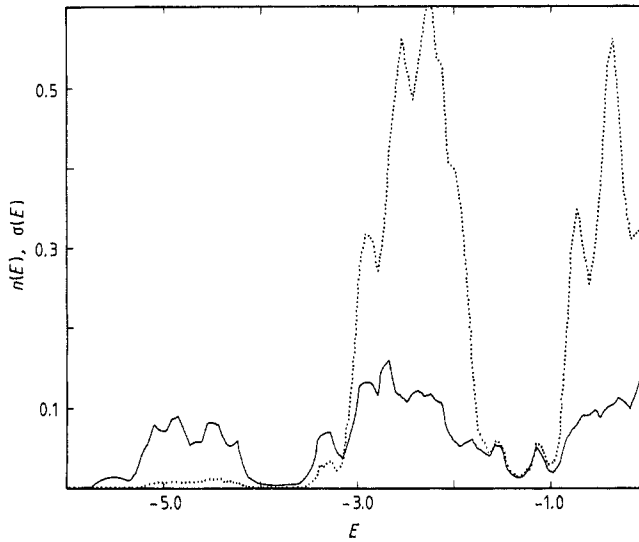
$$n(E)^{2D} = \int n(E - \lambda)^{1D} n(\lambda)^{1D} d\lambda$$

$$\sigma(E)^{2D} = \int \sigma(E - \lambda)^{1D} n(\lambda)^{1D} d\lambda.$$
(21)

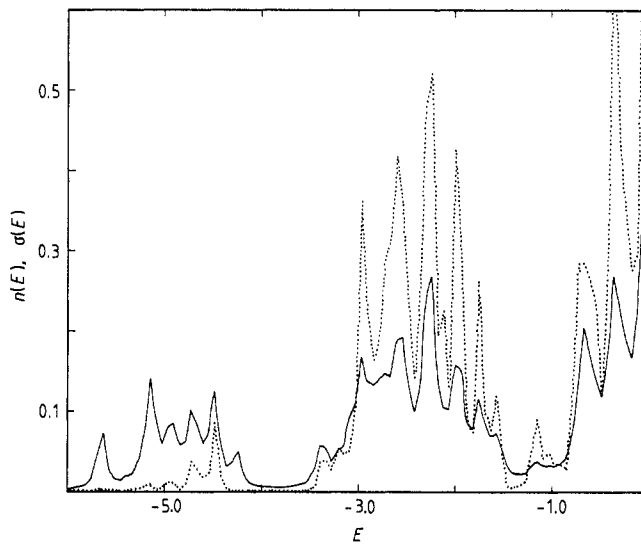
A similar idea was used in [14] to construct 2D models for vibrational motion in glasses.

We have performed the convolutions numerically using the 1D results for  $n(E)$  and  $\sigma(E)$  shown in figure 5. The results are shown in figure 6 and can be used to compare with those obtained using the recursion method as explained in § 2.3. The density of states of this 2D example has three sub-bands in the region of negative energies and a large peak at  $E = 0$ , similar to a periodic square lattice, owing to the symmetry with respect to the permutation of  $x$  and  $y$ . The states of the lower sub-band must be localised because they arise as a direct product of the 1D localised states.

For the recursion 2D calculation, we have used a maximum of 40 levels in the continued fraction ( $N = 40$ ) to avoid large computational costs. The imaginary part of the energy  $\eta$  was taken to be 0.05 (twice that used in the 1D calculations shown in figures 3 and 5) and the average was performed over 40 randomly selected sites. The result of this calculation is shown in figure 7, and comparison with figure 6 gives very good agreement if one disregards the spurious structure in the central sub-band given by the



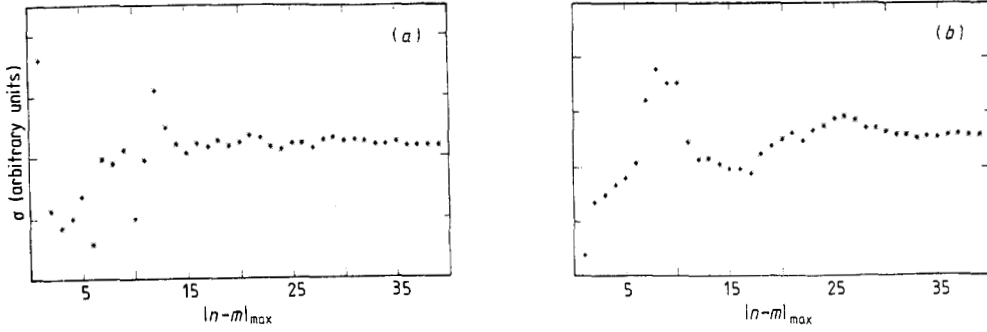
**Figure 6.** Density of states and conductivity for the 2D example obtained by numerical integration of equations (21). The starting 1D system is that in figure 5.



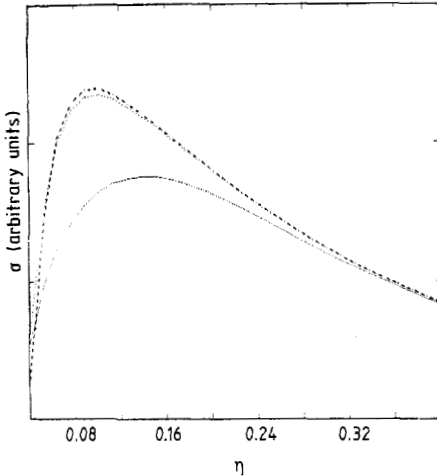
**Figure 7.** Density of states and conductivity for the 2D example calculated using the recursion basis as described in § 2.3.

recursion procedure. We expect that a larger number of recursion steps will as usual increase the number and decrease the magnitude of the oscillations.

In this calculation, we have neglected the matrix elements  $\langle v_n | C_x | v_m \rangle$  when  $|n - m|$  is large enough, as already mentioned in § 2.3. To prove that this is a good approximation, we show in figure 8 the contribution from one site to the conductivity as a function of the cut-off  $|n - m|_{\max}$  for two different energies. It is clear that the convergence is better for  $E = -4.9$ , where the states are expected to be localised but, in both cases,  $|n - m|_{\max}$



**Figure 8.** Conductivity as a function of the cut-off  $|n - m|_{\max}$  in the matrix elements  $\langle v_n | C_x | v_m \rangle$  for the 2D example for (a)  $E = -4.9$  and (b)  $E = -0.6$ .



**Figure 9.** Conductivity as a function of  $N$  and  $\eta$  for the 2D example and  $E = -4.9$ : —,  $N = 20$ ; ----,  $N = 30$ ; ...,  $N = 40$ . The lines for  $N = 30$  and  $N = 40$  are almost superimposed.

can be taken as 20 with an error of less than 10%. This allows us to increase the number of recursion steps, because fewer vectors must be stored simultaneously.

Finally, in order to confirm the expected character of the wavefunctions at the lower band in the 2D example, we studied the behaviour of  $\sigma$  against  $\eta$  for different values of  $N$ . The results, shown in figure 9, indicate the existence of localised states.

#### 4. Conclusions

We have proposed a new algorithm to calculate the conductivity of disordered systems based on the recursion method. The results obtained for 1D and 2D examples are encouraging as they show that the method is useful and numerically efficient.

The application of this formalism to 3D disordered systems (metals or semiconductors) is a natural extension of this work.

## Acknowledgment

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