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The Calculation of Transport Properties and Density of States of Disordered Solids

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A computational method is presented for the calculation of the conductivity tensor and the density of states of disordered solids. This is a more general and detailed discussion of an algorithm which has been applied to d.c. and a.c. conductivity, Hall effect and density of states of various systems.

1. Introduction

In the study of non-crystalline solids the lack of any simplifying symmetry poses a major problem in the calculation of electronic and other properties. Transport studies have proven particularily tricky since long range correlations and non-local contributions can play an important role.

In the simulation of such systems computer storage is usually the most significant limiting factor. For a system of N atoms diagonalisation requires the storage of $\approx N^2$ quantities; thus prohibiting the study of 3-dimensional systems of more than 5^3 atoms.

Some methods have been developed which have a storage requirement $\propto N$ which allows up to 25^3 atoms. The *recursion* method [1] and the *equation of motion* method [2, 3] have proven useful for the calculation of densities of states and related properties. Transport properties have proven more elusive however [4, 5].

In this paper an algorithm will be presented which contains no limitation due to computer storage on the volume of the systems which can be treated. $N \approx 10^9$ has been considered. The systems are very anisotropic however: $N = M^{d-1}L$ where $M^{d-1} < 100$ and L is essentially unbounded. While this may be a disadvantage in a few cases, it is generally possible to increase L sufficiently to achieve a very accurate result whose dependence on M can be studied [6, 7].

This paper will deal with a very general form of the algorithm, for which particular cases have been considered by various authors.

2. The Basic Algorithm

Consider a *tight-binding* Hamiltonian of the form

$$\mathscr{H} = \sum_{ij} H_{ij} |i\rangle \langle j| \tag{1}$$

where the functions $|i\rangle$ are located at points on a regular lattice and $\mathscr{H}$ is hermitian but otherwise general. For simplicity let us consider all matrix elements H_{ij} where i and j are not on the same or nearest neighbour sites to be zero.

Any lattice can be divided into *slices* along one lattice direction such that each slice may be labelled by a single integer, Fig. 1. The system we consider here will be built up of a large number of such slices where each slice has a finite cross-section, with periodic or free boundary conditions.

In what follows all quantities written in **BOLD CAPITALS** are matrices operating in the subspace of a slice and the indices refer to slices. In this way a

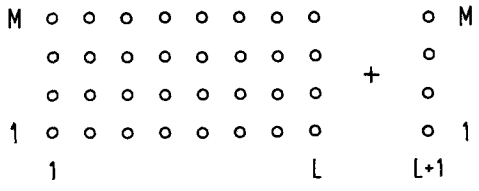

Fig. 1. Schematic picture of the iterative procedure used for the calculation of ρ, σ_{xx} and σ_{xy}. A quantity corresponding to a system of size $(L+1)\cdot M$, $\mathbf{A}^{(L+1)}$, is related to the same quantity for the system of size $L \cdot M$, $\mathbf{A}^{(L)}$ via a recursive relation $\mathbf{A}^{(L+1)} = f(\mathbf{A}^{(L)})$

Green's Function may be defined from

$$[\mathbf{Z}-\mathbf{H}_{ij}]\mathbf{G}_{ij}-\mathbf{H}_{i,j+1}\mathbf{G}_{i+1,j}-\mathbf{H}_{i,i-1}\mathbf{G}_{i-1,j}=\mathbf{I}\delta_{ij} \quad (2)$$

where $\mathbf{Z}=(E+i\gamma)\mathbf{I}$ is the complex energy.
Now consider a *stack* of *N-slices*. We wish to find the effect of adding an additional slice. The Hamiltonian may be divided into three contributions:

$$\mathscr{H}=\mathbf{H}_{ij}+(\mathbf{V}_N+\mathbf{V}_N^\dagger)+\mathbf{H}_{N+1}^0 \quad (3)$$

where $i,j\leqq N$, $\mathbf{V}_N=\mathbf{H}_{N,N+1}$ is the off-diagonal part coupling the N*th* and the $(N+1)$*st* slice, and $\mathbf{H}_{N+1}^0=\mathbf{H}_{N+1,N+1}$. We can calculate the Green's function for the $N+1$ slice system from that for the N slice system by using Dyson's equation with $\mathbf{V}_N$ as the interaction. Thus

$$\mathbf{G}_{ij}^{(N+1)}=\mathbf{G}_{ij}^{(N)}+\mathbf{G}_{iN}^{(N)}\mathbf{V}_N\mathbf{G}_{N+1,j}^{(N+1)}. \quad (4)$$

In particular

$$\mathbf{G}_{N+1,N+1}^{(N+1)}=[\mathbf{Z}-\mathbf{H}_{N+1}^0-\mathbf{V}_N^\dagger\mathbf{G}_{NN}^{(N)}\mathbf{V}_N]^{-1} \quad (5a)$$

$$\mathbf{G}_{ij}^{(N+1)}=\mathbf{G}_{ij}^{(N)}+\mathbf{G}_{iN}^{(N)}\mathbf{V}_N\mathbf{G}_{N+1,N+1}^{(N+1)}\mathbf{V}_N^\dagger\mathbf{G}_{Nj}^{(N)} \quad (i,j\leqq N) \quad (5b)$$

$$\mathbf{G}_{i,N+1}^{(N+1)}=\mathbf{G}_{iN}^{(N)}\mathbf{V}_N\mathbf{G}_{N+1,N+1}^{(N+1)} \quad (i\leqq N) \quad (5c)$$

$$\mathbf{G}_{N+1,j}^{(N+1)}=\mathbf{G}_{N+1,N+1}^{(N+1)}\mathbf{V}_N^\dagger\mathbf{G}_{Nj}^{(N)} \quad (j\leqq N). \quad (5d)$$

In this way we can generate any element of the Green's function for the new system and we can build a stack of any thickness by starting from a single slice and repeatedly applying (5).
In the following discussion we shall require both advanced and retarded Green's functions, $\mathbf{G}^-$ and $\mathbf{G}^+$. For a hermitian Hamiltonian these are related by

$$\mathbf{G}_{ij}^-=(\mathbf{G}_{ji}^+)^\dagger. \quad (6)$$

3. The Density of States and Conductivity Tensor

In this section we shall derive formulae for the density of states, ρ, and for the diagonal and off-diagonal components of the conductivity tensor, σ_{xx} and σ_{xy}. These may be defined as follows [8]:

$$\rho(E)=\frac{-1}{\pi NM}\operatorname{Im}\sum_{i=1}^{N}\operatorname{Tr}\mathbf{G}_{ij}^+ \quad (7a)$$

$$\sigma_{xx}=\frac{e^2}{h}\frac{4}{NM}\operatorname{Tr}\left\{\gamma^2\sum_{ij}^{N}\mathbf{G}_{ij}^+x_j\mathbf{G}_{ji}^-x_i - i\gamma\tfrac{1}{2}\sum_i^N(\mathbf{G}_{ii}^+-\mathbf{G}_{ii}^-)x_i^2\right\} \quad (7b)$$

$$\sigma_{xy}=\frac{e^2}{h}\frac{4}{NM}\operatorname{Tr}\left\{\gamma^2\sum_{ij}^{N}\mathbf{G}_{ij}^+\mathbf{y}\mathbf{G}_{ji}^-x_i - i\gamma\tfrac{1}{2}\sum_i^N(\mathbf{G}_{ii}^+-\mathbf{G}_{ii}^-)x_i\mathbf{y}\right\} \quad (7c)$$

where the $\mathbf{G}_{ij}$ are evaluated at the Fermi energy E_F, M is the cross-section of a slice, $\mathbf{y}$ is the diagonal operator representing the position accross the slice and x_i is the (scalar) position of the i^{th} slice.
We are now in a position to derive recursion formulae by substituting (5) into (7). The results are expressed in terms of the following ancillary matrices for the stacks of N-slices:

$$\mathbf{R}_N=\mathbf{G}_{NN}^+ \quad (8a)$$

$$\mathbf{A}_N=\gamma\mathbf{V}_N^\dagger\left[\sum_{ij}^{N}\mathbf{G}_{Nj}^+\mathbf{y}(2\gamma\mathbf{G}_{ji}^- - i\mathbf{I}\delta_{ij})x_i\mathbf{G}_{iN}^+\right]\mathbf{V}_N \quad (8b)$$

$$\mathbf{B}_N=\gamma\mathbf{V}_N^\dagger\left[\sum_{ij}^{N}\mathbf{G}_{Nj}^+x_j(2\gamma\mathbf{G}_{ji}^- - i\mathbf{I}\delta_{ij})x_i\mathbf{G}_{iN}^+\right]\mathbf{V}_N \quad (8c)$$

$$\mathbf{C}_N^+=\gamma\mathbf{V}_N^\dagger\left[\sum_{i}^{N}\mathbf{G}_{Ni}^+x_i\mathbf{G}_{iN}^-\right]\mathbf{V}_N=(\mathbf{C}_N^+)^\dagger \quad (8d)$$

$$\mathbf{C}_N^-=\gamma\mathbf{V}_N^\dagger\left[\sum_{i}^{N}\mathbf{G}_{Ni}^-x_i\mathbf{G}_{iN}^+\right]\mathbf{V}_N=(\mathbf{C}_N^-)^\dagger \quad (8e)$$

$$\mathbf{D}_N=\gamma\mathbf{V}_N^\dagger\left[\sum_{i}^{N}\mathbf{G}_{Ni}^+\mathbf{y}\mathbf{G}_{iN}^-\right]\mathbf{V}_N=(\mathbf{D}_N)^\dagger \quad (8f)$$

$$\mathbf{F}_N=\mathbf{V}_N^\dagger\left[\sum_{i}^{N}\mathbf{G}_{Ni}^+\mathbf{G}_{iN}^+\right]\mathbf{V}_N. \quad (8g)$$

In deriving the recursion relations we consider the new slice to be at $x_{N+1}=0$ (see end of this section). This considerably simplifies the equations. By combining (5), (7) and (8) we obtain the relations:

$$s_\rho^{(N+1)}=s_\rho^{(N)}+\operatorname{Tr}\{\mathbf{R}_{N+1}\mathbf{F}_N\} \quad (9a)$$

$$s_{xx}^{(N+1)}=s_{xx}^{(N)}+\operatorname{Tr}\{\operatorname{Re}(\mathbf{B}_N\mathbf{R}_{N+1}) + \mathbf{C}_N^+\mathbf{R}_{N+1}^\dagger\mathbf{C}_N^-\mathbf{R}_{N+1}\} \quad (9b)$$

$$s_{xy}^{(N+1)}=s_{xy}^{(N)}+\operatorname{Tr}\{\operatorname{Re}(\mathbf{A}_N\mathbf{R}_{N+1}) + (\mathbf{D}_N+\gamma\mathbf{y})\mathbf{R}_{N+1}^\dagger\mathbf{C}_N^-\mathbf{R}_{N+1}\} \quad (9c)$$

$$\mathbf{R}_{N+1}=[\mathbf{Z}-\mathbf{H}_{N+1}^0-\mathbf{V}_N^\dagger\mathbf{R}_N\mathbf{V}_N]^{-1} \quad (9d)$$

$$\mathbf{A}_{N+1}=\mathbf{V}_{N+1}^\dagger\mathbf{R}_{N+1}[\mathbf{A}_N+2(\mathbf{D}_N+\gamma\mathbf{y})\mathbf{R}_{N+1}^\dagger\mathbf{C}_N^-] \cdot\mathbf{R}_{N+1}\mathbf{V}_{N+1} \quad (9e)$$

$$\mathbf{B}_{N+1}=\mathbf{V}_{N+1}^\dagger\mathbf{R}_{N+1}[\mathbf{B}_N+2\mathbf{C}_N^+\mathbf{R}_{N+1}^\dagger\mathbf{C}_N^-]\mathbf{R}_{N+1}\mathbf{V}_{N+1} \quad (9f)$$

$$\mathbf{C}_{N+1}^+=\mathbf{V}_{N+1}^\dagger\mathbf{R}_{N+1}\mathbf{C}_N^+\mathbf{R}_{N+1}^\dagger\mathbf{V}_{N+1} \quad (9g)$$

$$\mathbf{C}_{N+1}^-=\mathbf{V}_{N+1}^\dagger\mathbf{R}_{N+1}^\dagger\mathbf{C}_N^-\mathbf{R}_{N+1}\mathbf{V}_{N+1} \quad (9h)$$

$$\mathbf{D}_{N+1}=\mathbf{V}_{N+1}^\dagger\mathbf{R}_{N+1}(\mathbf{D}_N+\gamma\mathbf{y})\mathbf{R}_{N+1}^\dagger\mathbf{V}_{N+1} \quad (9i)$$

$$\mathbf{F}_{N+1}=\mathbf{V}_{N+1}^\dagger\mathbf{R}_{N+1}(\mathbf{F}_N+\mathbf{I})\mathbf{R}_{N+1}\mathbf{V}_{N+1} \quad (9j)$$

From these we can write

$$\rho^{(N)}=\frac{-1}{\pi NM}\,\mathrm{Im}\,s_{\rho}^{(N)} \tag{10a}$$

$$\sigma_{xx}^{(N)}=\frac{e^2}{h}\,\frac{4}{NM}\,s_{xx}^{(N)} \tag{10b}$$

$$\sigma_{xy}^{(N)}=\frac{e^2}{h}\,\frac{4}{NM}\,s_{xy}^{(N)}. \tag{10c}$$

There is one additional correction to be added. Although the conductivities are independent of the choice of origin for x_i the matrices $\mathbf{A}_N$, $\mathbf{B}_N$ and $C_N^{\pm}$ are not. However it is possible to shift the origin of x_i at each stage to the position of the current slice. By substituting $x_i \to x_i - 1$ in (8) and using the identity

$$\gamma\sum_{i}^{N}\mathbf{G}_{Ni}^{+}\mathbf{G}_{iN}^{-}=i\tfrac{1}{2}(\mathbf{G}_{NN}^{+}-\mathbf{G}_{NN}^{-}) =i\tfrac{1}{2}(\mathbf{R}_N-\mathbf{R}_N^{\dagger}) \tag{11}$$

the required conditions become

$$\mathbf{A}_N'=\mathbf{A}_N+i\mathbf{D}_N \tag{12a}$$

$$\mathbf{B}_N'=\mathbf{B}_N+i\mathbf{C}_N^{+}+i\mathbf{C}_N^{-}+\tfrac{1}{2}\mathbf{V}_N^{\dagger}(\mathbf{R}_N-\mathbf{R}_N^{\dagger})\mathbf{V}_N \tag{12b}$$

$$\mathbf{C}_N^{\pm\prime}=\mathbf{C}_N^{\pm}-i\tfrac{1}{2}\mathbf{V}_N^{\dagger}(\mathbf{R}_N-\mathbf{R}_N^{\dagger})\mathbf{V}_N. \tag{12c}$$

This correction has the additional numerical advantage that it eliminates terms like $(x_i+1)^2-x_i^2$ which can give rise to numerical instability for large x_i. It is more generally applicable than the procedure discussed by Saso [9] for a purely 1-dimensional system.

4. Boundary Conditions

There are two types of boundary conditions which must be considered:

i) accross each slice

ii) at the beginning and end of the stack.

For ρ and σ_{xx} periodic boundary conditions accross the slices are usually to be preferred, so that the strip becomes a cylinder. In the case of σ_{xy}, however, this choice is not available due to the presence of the **y** operator in (7c). In this case the simplest choice is free boundary conditions. This may not be the best choice however (see Sect. 5).

The choice of boundary conditions at the ends is more complicated. We should like to make the system effectively infinitely large so that we can set the parameter γ to zero. This can be accomplished by adding semi-infinite ideal metals to both ends, with the operator, x, defined to be constant in the metallic part. We may do this since the electric field should be zero in the metal and current conservation ensures that the current calculated in the disordered part alone is the same as the current in the metals.

The equation for the Green's function on an ordered stack may be written in the form

$$\begin{bmatrix}\mathbf{V} & \mathbf{0}\\ \mathbf{0} & \mathbf{V}^{\dagger-1}\end{bmatrix}\begin{bmatrix}\mathbf{G}_{i+1,j}\\ \mathbf{V}^{\dagger}\mathbf{G}_{ij}\end{bmatrix} =\begin{bmatrix}\mathbf{Z}-\mathbf{H} & -\mathbf{I}\\ \mathbf{I} & \mathbf{0}\end{bmatrix}\begin{bmatrix}\mathbf{G}_{ij}\\ \mathbf{V}^{\dagger}\mathbf{G}_{i-1,j}\end{bmatrix}-\begin{bmatrix}\delta_{ij}\\ \mathbf{0}\end{bmatrix}. \tag{13}$$

To solve this for **G** we must first consider the general eigenvalue problem

$$\alpha\begin{bmatrix}\mathbf{V} & \mathbf{0}\\ \mathbf{0} & \mathbf{V}^{\dagger-1}\end{bmatrix}\begin{bmatrix}\mathbf{U}^a\\ \mathbf{U}^b\end{bmatrix}=\begin{bmatrix}\mathbf{Z}-\mathbf{H} & -\mathbf{I}\\ \mathbf{I} & \mathbf{0}\end{bmatrix}\begin{bmatrix}\mathbf{U}^a\\ \mathbf{U}^b\end{bmatrix} \tag{14}$$

where α is the eigenvalue and **U** is the matrix of eigenvectors.

For $i<j$ the columns of $\mathbf{G}_{ij}$ are linear combinations of those columns of $\mathbf{U}^a$ corresponding to eigenvalues with $|\alpha|>1$:

$$\mathbf{G}_{ij}=\mathbf{U}^a\underline{\alpha}^{i-j}\mathbf{A} \tag{15}$$

where $\underline{\alpha}$ is the diagonal matrix of such eigenvalues. From this $\mathbf{G}_{00}$ at the end of a semi-infinite $(-\infty\to 0)$ stack can be found by solving

$$\mathbf{V}\mathbf{G}_{10}=\mathbf{V}\mathbf{U}^a\underline{\alpha}\mathbf{A}=\mathbf{I} \quad (|\alpha|>1) \tag{16}$$

so that

$$\mathbf{G}_{00}^{-\infty}=\mathbf{U}^a\underline{\alpha}^{-1}[\mathbf{U}^a]^{-1}\mathbf{V}^{-1} \quad (|\alpha|>1). \tag{17}$$

Similarly the result for a $(0\to\infty)$ stack is

$$\mathbf{G}_{00}^{+\infty}=\mathbf{U}^a\underline{\alpha}[\mathbf{U}^a]^{-1}[\mathbf{V}^{\dagger}]^{-1}=\mathbf{S}_{\infty}^{-1} \quad (|\alpha|<1) \tag{18}$$

where $\mathbf{S}_{\infty}$ is the corresponding self-energy matrix which will be required later.

Since we can define $x_i=0$ at the beginning and at the end the initial values of **A**, **B**, $\mathbf{C}^{\pm}$ are zero. The matrix **F** may also be defined to be zero since the sum over i only runs over the disordered region. Thus for ρ and σ_{xx} the only changes required are to use $\mathbf{G}_{00}^{-\infty}$ as the initial value of **R** and to add a slice characterised by $\mathbf{S}_{\infty}$ to the leading end. Note that it is not necessary to do the latter operation after each slice but only when it is desired to print out the results.

In the case of σ_{xy} the matrix **D** must be calculated for the semi-infinite stacks. By choosing $\mathbf{Z}=(E-i\gamma)\mathbf{I}$ in (14) (**R** can still be calculated using (6)) we can write

$$\mathbf{D}^{-\infty} = \gamma \mathbf{V}^{\dagger} \sum_{n=0}^{\infty} \mathbf{A}^{\dagger}(\underline{\alpha}^{*})^{-n} \mathbf{U}^{\dagger} \mathbf{y} \mathbf{U} \underline{\alpha}^{-n} \mathbf{A} \mathbf{V} \quad (|\alpha| > 1) \tag{19a}$$

$$D_{ij}^{-\infty} = \sum_{kl} [\mathbf{AV}]_{ki}^{*} [\mathbf{U}^{\dagger} \mathbf{y} \mathbf{U}]_{kl} [\mathbf{AV}]_{lj} \left\{ \frac{\gamma \alpha_k^* \alpha_l}{\alpha_k^* \alpha_l - 1} \right\} \tag{19b}$$

for a $(-\infty \to 0)$ stack and

$$D_{ij}^{+\infty} = \sum_{kl} [\mathbf{AS}_{\infty}]_{ki}^{*} [\mathbf{U}^{\dagger} \mathbf{y} \mathbf{U}]_{kl} [\mathbf{AS}_{\infty}]_{lj} \left\{ \frac{\gamma}{1 - \alpha_k^* \alpha_l} \right\}$$

$$(|\alpha| < 1) \tag{20}$$

for $(0 \to \infty)$. In these formulae $[\ ]_{ij}$ refers to the ijth element of the matrix in the square brackets $[\ ]$.
Thus the initial value of $\mathbf{D}$ is given by $\mathbf{D}^{-\infty}$ and $\mathbf{D}^{+\infty}$ must be added to $\mathbf{D}_N$ in (9c).

5. Finite Size Effects in σ_{xy}

If we rewrite the definition of σ_{xy} for a 2-dimensional strip of width M in terms of extensive variables we obtain

$$I_x = \sigma_{xy} \Delta V_y \tag{21}$$

where I_x is the total current flowing through the stack (i.e. $I_x = J_x M$ where J_x is the current density) and ΔV_y is the potential difference accross each slice. Unfortunately for a lattice system of finite size ΔV_y is not well defined since the two points between which the difference is to be measured have not been defined. In fact the correct definition must involve the expectation values of the potential V of two or more states associated with opposite sides of the system. Thus the effective length associated with ΔV will be less than the total width of the system by a factor ΔM which may be a sensitive function of the details of the eigenstates. The calculated value of σ_{xy} will be in error by a factor $\dfrac{M - \Delta M}{M}$.
This may be overcome in one of two ways. The simplest way is to redefine the operator $\mathbf{y}$ to have the value $-\frac{1}{2}M$ in one half of the slice and $+\frac{1}{2}M$ in the other. Often, e.g. for the Quantum Hall Effect [8], the result does not depend on the detailed behaviour of the electric field but only on $\Delta V (= M)$ the potential difference accross the system.
A more complex way of correcting the error, and one more in line with the real experimental situation, consists of attaching semi-infinite one-dimensional wires to all edge atoms. In these wires, as in those attached to the ends of the strip, the potential may be treated as constant and equal to the maximum or minimum values $(\pm\frac{1}{2}M)$ at the respective edges.

The Green's function g at the end of such a semi-infinite $1-D$ wire can be written in the form

$$g = \frac{Z \pm \sqrt{Z^2 - 4|V|^2}}{2|V|^2} \tag{22}$$

where the sign of the square root is chosen so that the $\mathrm{Im} g$ has the opposite sign to $\mathrm{Im} Z$, and V is the off-diagonal element between the neighbouring atoms of the wire.
When the chain is attached to the edge of our stack the result may be expressed in terms of a self-energy correction

$$s = |V|^2 g \tag{23}$$

to the atoms on the edges of the stack. In addition the terms $\gamma \mathbf{y}$ in (9) must be modified by the addition of a term $-\mathbf{y}_{\min}^{\max} \mathrm{Im} s$ to the contributions from the edges.
In general neither Z nor V must be the same as in the bulk stack so that we are free to choose $s = \pm i\eta$ for the self-energy.
It is worth noting at this point that in the limit $\gamma \to 0$ only these contributions survive (see Eqs. (9)); thus confirming that the detailed behaviour of the applied potential is unimportant.

6. The Limit $\gamma \to 0$

Although it is possible to interpret the parameter γ as having physical meaning (lifetime, inelastic scattering time, etc.) we would nevertheless like to be able to eliminate γ from the above algorithm.
Interestingly, although the definitions in (7) and (8) contain γ, the recursion relations (9), (10), (12) do not, except in the form $\gamma \mathbf{y}$ as discussed above. The only part of the algorithm where special care is required is in the treatment of the semi-infinite metals at the ends. When $\gamma = 0$ the eigenvalues, α, of (14) can have modulus unity, $|\alpha| = 1$, so that the division into groups with $|\alpha| > 1$ or $|\alpha| < 1$ is no longer unambiguous. Care is also required with the terms in curly brackets $\{\ \}$, in (19) and (20).
Whenever $|\alpha| = 1$ it is necessary to consider the derivative $\dfrac{d\alpha}{d\gamma}$ in order to resolve the ambiguity. Ignoring the (unlikely) possibility that the α are degenerate we can write

$$\frac{d\alpha}{d\gamma} = i \frac{\mathbf{u}_L^a \cdot \mathbf{u}_R^a}{\mathbf{u}_L^a \mathbf{V} \mathbf{u}_R^a + \mathbf{u}_L^b [\mathbf{V}^{\dagger}]^{-1} \mathbf{u}_R^b} \tag{24}$$

where the $\mathbf{u}_L^{a,b}$ and $\mathbf{u}_R^{a,b}$ are the left and right handed eigenvectors corresponding to α.

Thus we may conclude that $|\alpha|>1$ if $\mathrm{Re}\left(\alpha^* \frac{d\alpha}{d\gamma}\right)>0$ and vice versa. With this information we can choose the correct contributions to (15)–(18).

Again assuming that the α are non-degenerate, the terms in curly brackets, { }, in (19b) and (20) become

$$\left\{\frac{\gamma \alpha_k^* \alpha_l}{\alpha_k^* \alpha_l - 1}\right\} \to \frac{\delta_{kl}}{2\,\mathrm{Re}\left(\alpha_k^* \frac{d\alpha_k}{d\gamma}\right)} \qquad (|\alpha_k|=1) \qquad (25a)$$

$$\to 0 \qquad (|\alpha_k| \neq 1) \qquad (25b)$$

and

$$\left\{\frac{\gamma}{1-\alpha_k^* \alpha_l}\right\} \to \frac{-\delta_{kl}}{2\,\mathrm{Re}\left(\alpha_k^* \frac{d\alpha_k}{d\gamma}\right)} \qquad (|\alpha_k|=1) \qquad (25c)$$

$$\to 0 \qquad (|\alpha_k| \neq 1) \qquad (25d)$$

respectively.

These terms illustrate a very important property of the ideal metals: namely that only those modes with $|\alpha|=1$ contribute to the transport. This is physically reasonable since only such modes can carry a current from $-\infty$ to $+\infty$.

A note of warning is necessary at this point. It is important that the ideal metals are defined in such a way that they are capable of carrying sufficient current at the chosen Fermi energy. In particular if this lies in a gap in the metals we will get $\rho=\sigma_{xx}=\sigma_{xy}=0$ since the metals have become insulators and no current can flow.

On the other hand, if the metals are too dissimilar to the disordered region of interest extra scattering contributions from the boundary may distort the result.

This problem can be overcome in principle by constructing an infinite chain of disordered blocks rather than the metal–disorder–metal configuration considered here [10].

Special Case σ_{xy}

When calculating σ_{xy} we can also consider infinitely weak coupling of the 1-dimensional wires discussed above. The parameter η which describes the coupling of these wires to the rest of the system must be larger than γ in order to be effective. η always appears as an additional contribution to γ either in the definition of the complex energy $\mathbf{Z}$ or in the term $\gamma\mathbf{y}$. Thus, when $\gamma \gg \eta$, η can be neglected and, when $\eta \gg \gamma$, γ can be neglected. This implies however that we may set γ to zero and simply consider the limit $\eta \to 0$.

There are in fact very few modifications to the standard procedure which are required to take account of this. We can substitute η for γ everywhere and make two other changes:

i) $\mathbf{y} \to (y_{\min}, 0, \ldots, 0, y_{\max})$ everywhere, in particular in (19) and (20);

ii) $\mathbf{u}_L^a \cdot \mathbf{u}_R^a \to u_{L1}^a u_{R1}^a + u_{LM}^a u_{RM}^a$ in (24).

In this case the detailed behaviour of $\mathbf{y}$ and the electric field is no longer required. Only the extreme values of $\mathbf{y}$ survive, which represent the potential difference between the $1-D$ wires at opposite sides of the system. This is, of course, exactly the quantity measured in an experiment.

7. Some Special Cases, the Effects of Symmetry

When the Hamiltonian contains some symmetry certain of the recursion relations simplify. A common example is when the Hamiltonian is real. Then the Green's function is symmetric and this symmetry also applies to $\mathbf{R}_N$, $\mathbf{B}_N$ and $\mathbf{F}_N$. In addition $\mathbf{C}_N^+ = \mathbf{C}_N^-$ and the conductivity tensor is symmetric ($\sigma_{xy}=\sigma_{yx}$).

In (14) when $\mathbf{H}$ and $\mathbf{V}$ are symmetric the left hand eigenvectors are related to the right hand ones by

$$[\mathbf{U}_L^a, \mathbf{U}_L^b] = [\mathbf{U}_R^{aT}, -\mathbf{U}_R^{bT}] \qquad (26)$$

which considerably simplifies the perturbation theory, (24). This condition is rather weaker than that the Hamiltonian of the whole system is real.

When the matrices $\mathbf{V}$ between the slices of the stack can be expressed as the product of a scalar and a unit matrix the $\mathbf{V}$'s can be eliminated from all recursion relations.

In most cases of interest the ideal metals can be defined such that (14) can be solved analytically by using Bloch's theorem, thus saving considerable computational work.

8. Discussion

Algorithms of the type discussed in detail in this paper have been successfully applied to the study of the d.c. conductivity of one dimensional disordered systems [11] and more recently to the a.c. conductivity [9. 12]. The generalisation to disordered strips and bars [13] has recently been successfully applied to systems in a magnetic field including the study of ρ, σ_{xx} and σ_{xy} in connection with the Quantum Hall Effect [8, 14, 15].

Generalisations to diffusion [16] and to topological disorder [17] have also appeared.

The method is closely related to that employed in the study of Anderson localisation in disordered systems [6, 7, 14].

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