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The Kubo formula for the conductance of finite systems in the ballistic regime: a simple algorithm

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Abstract. We present a method for obtaining the conductance within the linear response approximation of a disordered system of finite cross section described by a tight-binding Hamiltonian. This method is an extension of previous work in which we proposed a numerical algorithm for evaluating the Kubo formula in the spirit of the recursion method. We obtain simple recursive equations for the conductance that can be easily computed. As an application we study the problem of ballistic transport through a constriction using a confining model potential that allows us to investigate the dependence of the conductance quantisation as a function of Fermi energy, gate voltage and channel length. It is found that the conductance steps as a function of gate voltage are sensitive to the channel length. The possible extension of this work for use in studying the AC transport in these systems is briefly discussed.

1. Introduction

The problem of ballistic transport in small devices has recently received considerable attention. In particular, several theoretical studies of the conductance quantisation observed when narrow constrictions are imposed on a two-dimensional electron gas have been presented [1–7]. Most of these studies [1–4] are based on a Landauer-type picture for the conductance in which the transmission coefficients are calculated by matching the wave functions between regions in which the confining model potential is uniform. This approach may require a great deal of computing time when one wishes to study the effects of disorder or confining potentials of arbitrary shape.

On the other hand, a different approach based on linear response theory in a tight-binding representation was proposed by Mašek and Kramer [6]. In their formulation the non-locality effects associated with a finite system are included by considering a finite disordered region, where the driving electric field is constant, embedded in an infinite perfect conductor where the electric field vanishes. This approach has been shown to be equivalent to the Landauer picture in its simpler form [8], but it has the advantage that it can be generalised to give the AC conductance. We shall limit ourselves to this formulation in the following.

In previous work [9] (hereafter referred to as I) we proposed a numerical algorithm for evaluating the Kubo formula for the conductivity in a tight-binding model via a set of recursive equations. The key point of our procedure was to note that a generalised matrix form of Dyson's equation may be written for a product of Green functions that

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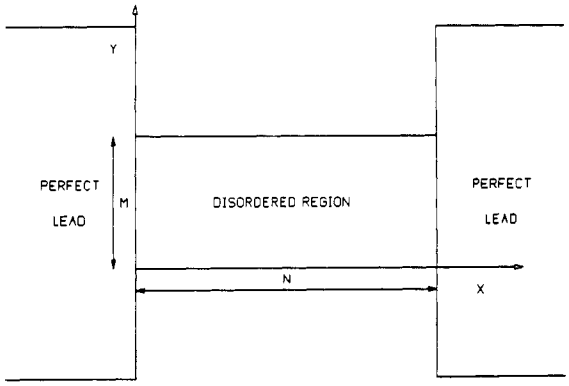

Figure 1. A schematic representation of the system considered.

essentially gives the conductivity. In the case of one-dimensional systems this leads to a continued fraction expansion of the relevant matrix elements, similar to what is found in the recursion method of Haydock [10].

The aim of the present work is to extend this idea to the case of strips or wires of finite cross section, so as to model the problem of transport in mesoscopic devices. As we show in the next section, the simplicity of the recursive equations that arise from the present formalism makes it convenient when compared to previous methods, such as those presented in [11] and [12].

On the other hand, as an application of our method, we present some new results for the conductance through a narrow channel in which we have investigated the effects of a non-uniform model potential.

2. Formalism for the conductance

We consider a tight-binding Hamiltonian on a two-dimensional square lattice. For simplicity we assume interactions only between first neighbours with a fixed value for all sites, taken as the unit of energy. The lattice constant is taken as the unit of length. Only the on-site elements of the Hamiltonian are allowed to vary throughout the system.

We wish to obtain the DC conductance Γ_x in the x direction for a strip of width M and length N as indicated in figure 1. We assume free boundary conditions on the edges at $y = 0$ and $y = M$ and add perfect semi-infinite conductors to both ends at $x = 0$ and $x = N$. As in I, we define first the operators:

$$C_x = [x, H] \tag{1}$$

and

$$S(z_1, z_2) = G(z_1)C_xG(z_2) \tag{2}$$

where $G(z) = (z - H)^{-1}$ is the Green function operator. On making this replacement in the Kubo formula, the conductance at zero temperature is given by

$$\Gamma_x(E) = (2e^2/hN^2)\,\mathrm{Tr}[C_x\,\mathrm{Re}(S^+(E) - S^-(E))] \tag{3}$$

where Tr denotes trace operation, E is the Fermi energy and $S^{\pm}(E) = \lim_{\eta\to 0} S(E + i\eta, E \pm i\eta)$.

We assume that the position operator in (1) is restricted to the sites on the disordered region, which is equivalent to taking the applied electric field as zero at the perfect leads attached to the strip [11]. Note that the particular choice made for the boundary conditions allows us to take η effectively equal to zero [12].

For the case of a strip it is convenient to work with the projection operators defined as

$$P_j = \sum_{m=1}^{M} |jm\rangle\langle jm|$$

which project onto the subspace associated with a transverse layer at $x = j$. Then, we use the notation A_{jk} to refer to the projected operator $P_j A P_k$. In this way, equation (3) may be written as

$$\Gamma_x(E) = \frac{e^2}{hN^2} \sum_{j=1}^{N-1} \mathrm{Tr}[(S^+_{jj+1}(E) - S^+_{j+1j}(E)) - (S^-_{jj+1}(E) - S^-_{j+1j}(E))]. \quad (4)$$

The recursive equations for the conductance are obtained noticing that G and S satisfy a set of coupled integral equations. If we use the decomposition $H = h + V$, where h is the on-layer part of H, and V describes the coupling between contiguous layers, then

$$G(z) = g(z)(1 + VG(z)) \quad (5)$$

where $g(z) = (z - h)^{-1}$, and, making the replacement in (2),

$$S(z_1, z_2) = g(z_1)(C_x G(z_2) + VS(z_1, z_2)). \quad (6)$$

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

$$\mathbf{G}(z_1, z_2) = \mathbf{g}(z_1, z_2)(\mathbf{1} + \mathbf{VG}(z_1, z_2)) \quad (7)$$

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

$$\mathbf{g}(z_1, z_2) = \begin{pmatrix} g(z_2) & 0 \\ 0 & g(z_1) \end{pmatrix} \qquad \mathbf{G}(z_1, z_2) = \begin{pmatrix} G(z_2) & 0 \\ S(z_1, z_2) & G(z_1) \end{pmatrix} \qquad \mathbf{V} = \begin{pmatrix} V & 0 \\ C_x & V \end{pmatrix}.$$

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

$$\mathbf{G}_{ij}(z_1, z_2) = \begin{pmatrix} G_{ij}(z_2) & 0 \\ S_{ij}(z_1, z_2) & G_{ij}(z_1) \end{pmatrix}.$$

Equation (7) can now be solved recursively, in a way that is formally equivalent to the procedure described in I for a one-dimensional problem. The conductance is related to the matrix elements $S_{j,j+1}$, which are included in $\mathbf{G}_{j,j+1}$. These can be obtained if we

divide the strip in two semi-infinite regions: one starting from $x = j + 1$ to the right and the other from $x = j$ to the left. Then, from (7), we have

$$\mathbf{G}_{jj+1} = (\mathbf{1} - \mathbf{G}_j^{\mathrm{L}}\mathbf{V}_{\mathrm{LR}}\mathbf{G}_{j+1}^{\mathrm{R}}\mathbf{V}_{\mathrm{RL}})^{-1}\mathbf{G}_j^{\mathrm{L}}\mathbf{V}_{\mathrm{LR}}\mathbf{G}_{j+1}^{\mathrm{R}} \tag{8}$$

where

$$\mathbf{V}_{\mathrm{LR}} = \begin{pmatrix} \mathbf{1}_M & \mathbf{0} \\ \mathbf{1}_M & \mathbf{1}_M \end{pmatrix} \qquad \mathbf{V}_{\mathrm{RL}} = \begin{pmatrix} \mathbf{1}_M & \mathbf{0} \\ -\mathbf{1}_M & \mathbf{1}_M \end{pmatrix}$$

and $\mathbf{G}_j^{\mathrm{L}}$ and $\mathbf{G}_{j+1}^{\mathrm{R}}$ correspond to the surfaces of each of the semi-infinite regions and are given by the recursive matrix equations

$$\begin{aligned} \mathbf{G}_j^{\mathrm{L}} &= (\mathbf{1} - \mathbf{g}_j\mathbf{V}_{\mathrm{RL}}\mathbf{G}_{j-1}^{\mathrm{L}}\mathbf{V}_{\mathrm{LR}})^{-1}\mathbf{g}_j \\ \mathbf{G}_{j+1}^{\mathrm{R}} &= (\mathbf{1} - \mathbf{g}_{j+1}\mathbf{V}_{\mathrm{LR}}\mathbf{G}_{j+2}^{\mathrm{L}}\mathbf{V}_{\mathrm{RL}})^{-1}\mathbf{g}_{j+1}. \end{aligned} \tag{9}$$

The initial values for the iteration of equations (9) depend on the choice of the boundary conditions. In our case these must be

$$\mathbf{G}_0^{\mathrm{L}} = \mathbf{G}_{N+1}^{\mathrm{R}} = \begin{pmatrix} G_0(z_2) & 0 \\ 0 & G_0(z_1) \end{pmatrix}$$

with $G_0(z) = (z - h_0 - G_0(z))^{-1}$.

$G_0(z)$ is easily obtained if the eigenvectors of h_0 are known.

It is important to note that the perfect leads attached to the strip may have a width different from M, and thus the transition from a wide to a narrow channel may be modelled.

A fundamental point in our method is that the use of generalised operators gives a compact form to the recursive equations without introducing further difficulties into the computations. This is so because one has to deal with matrices of the form

$$\mathbf{A} = \begin{pmatrix} A_1 & 0 \\ A_3 & A_2 \end{pmatrix}$$

whose inverse $\mathbf{A}^{-1}$ is easily given in terms of A_1^{-1} and A_2^{-1} by

$$\mathbf{A}^{-1} = \begin{pmatrix} A_1^{-1} & 0 \\ -A_2^{-1}A_3A_1^{-1} & A_2^{-1} \end{pmatrix}.$$

Using this type of algebra, equations (9) can be expressed in terms of their matrix elements as

$$G_j^{\mathrm{L}}(z) = (z - h_j - G_{j-1}^{\mathrm{L}}(z))^{-1} \qquad G_{j+1}^{\mathrm{R}}(z) = (z - h_{j+1} - G_{j+2}^{\mathrm{R}}(z))^{-1}$$

$$S_j^{\mathrm{L}}(z_1, z_2) = G_j^{\mathrm{L}}(z_1)(S_{j-1}^{\mathrm{L}}(z_1, z_2) + G_{j-1}^{\mathrm{L}}(z_1) - G_{j-1}^{\mathrm{L}}(z_2))G_j^{\mathrm{L}}(z_2)$$

$$S_{j+1}^{\mathrm{R}}(z_1, z_2) = G_{j+1}^{\mathrm{R}}(z_1)(S_{j+2}^{\mathrm{R}}(z_1, z_2) + G_{j+2}^{\mathrm{R}}(z_1) - G_{j+2}^{\mathrm{R}}(z_2))G_{j+2}^{\mathrm{R}}(z_2). \tag{10}$$

Note that for $z_1 = z_2$, S_j^{L} and S_{j+1}^{R} are identically equal to zero for every j. Finally,

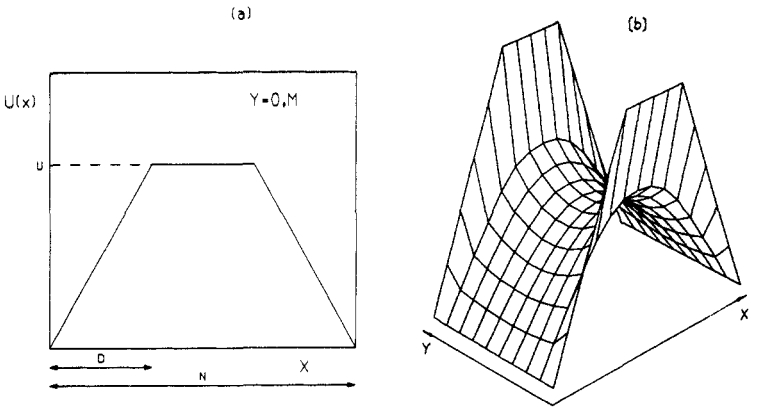

Figure 2. (*a*) Boundary values for the model potential for the channel at $y = 0$ and $y = M$. (*b*) The full shape of the potential.

the results obtained for G_j^{L}, G_{j+1}^{R}, S_j^{L} and S_{j+1}^{R} may be introduced in equation (8) and then, using (4), the complete expression for the conductance reduces to

$$\Gamma_x(E) = \frac{2e^2}{hN^2} \sum_{j=1}^{N-1} \mathrm{Re}\{\mathrm{Tr}[D_{jj+1}^{+}(G_j^{\mathrm{L}+} G_{j+1}^{\mathrm{R}+} - G_j^{\mathrm{L}+} G_{j+1}^{\mathrm{R}-} - S_j^{\mathrm{L}} G_{j+1}^{\mathrm{R}-} - G_j^{\mathrm{L}+} S_{j+1}^{\mathrm{R}}) D_{jj+1}^{-}]\} \tag{11}$$

where $D_{jj+1}(z) = (1 - G_j^{\mathrm{L}}(z) G_{j+1}^{\mathrm{R}}(z))^{-1}$.

To deduce expression (11) we have used the symmetry properties

$$(S_{jj+1}^{+})^{\dagger} = -S_{j+1j}^{+} \qquad (S_{jj+1}^{-})^{\dagger} = -(S_{j+1j}^{-})^{*}$$

that arise from the definition of the operator S.

An additional simplification to (11) comes from the fact that, in the DC limit, all terms in the sum are equal. This is a consequence of current conservation [8] and can be verified by algebraic manipulations. Thus, the more convenient choice is to take j at one of the ends of the strip ($j = 0$ or $j = N$).

3. Model calculations for the conductance through a constriction

Conductance quantisation is experimentally observed by imposing an 'electrostatic squeezing' onto a two-dimensional electron gas in a GaAs–AlGaAs heterojunction [13, 14]. In this technique a metal gate is deposited on top of the heterojunction and the width of the constriction is controlled by the application of a negative voltage to the gate.

In order to represent the effective potential for the electrons in the constriction we use the solutions of Laplace's equation for the strip with the following boundary conditions: we assume that the potential drops to zero on the perfect leads at $x = 0$ and $x = N$ and assume that it takes a value U, proportional to the gate voltage, at the edges on the y direction. The gate value U is not reached discontinuously, but there is a linear increase from 0 to U in a distance D, as shown in figure 2(*a*). The resulting model potential for the strip is plotted in figure 2(*b*).

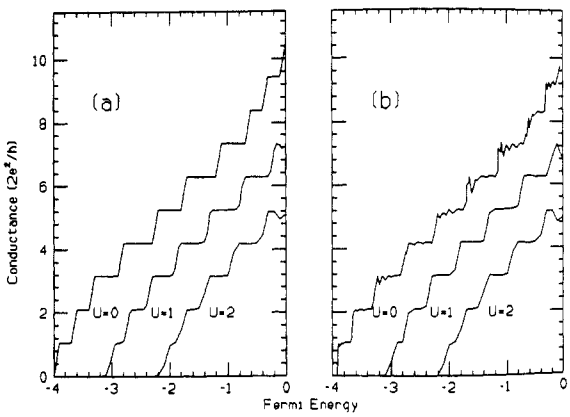

Figure 3. Conductance as a function of Fermi energy for $N = 21, M = 10, D = 6$ and different values of U. (a) Boundary leads of width M. (b) Boundary leads of width $2M$.

It is clear that this is only a rough approximation to the real potential as we are neglecting the screening by the electron gas. This will certainly reduce the electric field inside the channel and could be introduced in the model by means of an effective dielectric constant ε. However, we have verified that the results discussed below are not sensitive to this constant except for via a change in the U-scale.

We analyse first the dependence of the conductance on the width of the perfect leads at both ends of the strip. Figure 3(a) corresponds to the case where there is no discontinuity in the width (leads of width M). This figure plots the conductance against Fermi energy for different values of U. As expected, perfect quantisation occurs for $U = 0$ and the conductance steps become more rounded for increasing values of U. The same results but for boundary leads of width $2M$ are shown in figure 3(b). For $U = 0$ the conductance presents a resonant structure due to internal longitudinal reflections in the channel, as was also noted by other authors [1, 2]. Rather surprisingly these resonances are completely washed out for U different from zero. Comparing figures 3(a) and 3(b) we found that the width of the perfect leads plays no role in this case.

It is important to note that this particular dependence on the widths of the leads could be showing the limitations of the linear response approach. The qualitative analyses of this problem by Isawa [15] and Landauer [16] indicate that conductance quantisation is a property of electrons in a narrow channel connected to much wider leads, and that the conductance must diverge when the width of the leads is comparable to the channel width. This divergence does not appear within the linear approximation considered here.

We now discuss the results for the conductance as a function of U for fixed Fermi energy, in a way that can be more directly related to the experimental observations. The Fermi energy is fixed somewhere below and near the band centre ($E = 0$) where the effective mass is small. Figure 4 shows the last five or six steps before pinch off for different width to length (M/N) relations and D taken as $N/2$.

It can be seen that the step width is reduced as U increases for the case of a long channel ($N > M$), while the opposite behaviour is found for a short channel ($N \simeq M$). The observations of van Wees *et al* [13] correspond to this latter behaviour, which may be attributed to the particular geometry of the point contacts.

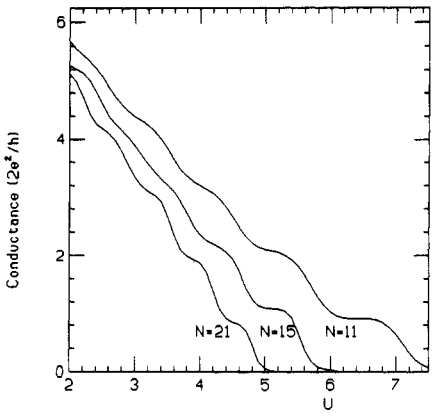

Figure 4. Conductance as a function of U for $E = -0.5$, $M = 10$ and D taken as $N/2$.

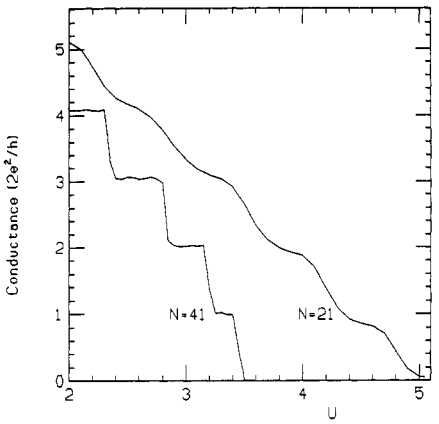

Figure 5. As figure 4, but for $D = 11$.

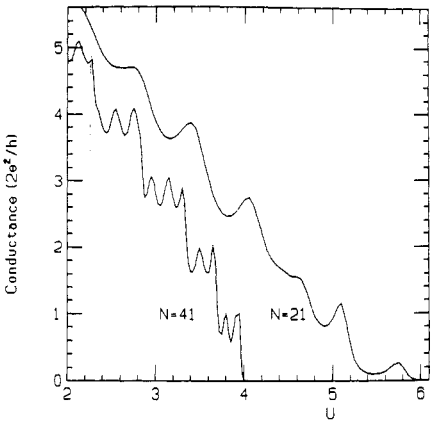

Figure 6. As figure 5, but for $E = 0$.

When N is increased for fixed M and D the potential tends to be more uniform both in the transverse and in the longitudinal directions, resulting in a better definition of the steps as shown in figure 5.

Finally we show in figure 6 similar results for $E_F = 0$. In this case, and also for higher Fermi energies, the steps are rather distorted by resonant peaks. These resonances cannot be simply analysed in terms of longitudinal reflections as they depend on the detailed form of the potential inside the channel. It should be possible to observe these effects provided that the electron density is varied by means of a dual gate device, such as those used in recent experiments on one-dimensional electrons [17, 18], but for channels short enough to ensure ballistic transport.

4. Conclusions

We have extended the ideas presented in I in order to calculate the conductance in the case of systems of finite section. Starting from a generalised matrix form of Dyson's

equation one arrives at a simple set of recursive equations for the conductance that can be solved by iteration. Each iteration is computationally equivalent to inverting a matrix whose dimensions depend on the width of the system considered. We found no problems of numerical instability using this procedure.

On the other hand, we have proposed a model for the quantum transport through a narrow constriction assuming that the potential for the electrons in the channel may be approximated by a solution of Laplace's equation. This model predicts quantised conductance steps as a function of gate voltage that are sensitive to the channel length and to the Fermi energy, as described in the previous section. These results help to clarify the relation between the qualitative shape of the observed conductance steps and the geometrical restrictions imposed on the electrons in the experimental devices.

The present formalism could be also used to study the AC transport in these systems. In particular, Mašek and Kramer [6] have demonstrated the appearance of oscillations in the AC conductance for freely propagating electrons. The object of future work will be to study whether these oscillations remain for a non-uniform potential.

We believe that, in spite of its limitations, the linear response approximation is useful for the study of ballistic transport in finite systems, since it provides a simple scheme for performing calculations that are in agreement with the available experimental data.

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