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Magnetoconductance in multiprobe systems

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Abstract. A flexible method is presented for calculating the conductance coefficients of small multiprobe devices in terms of real-space Green functions in a discretized space. Within the independent-particle approximation systems with arbitrary magnetic field and local potential can be dealt with. The method is based on a transparent analytical formula for the differential current flowing across an interface dividing the phase-coherent conductor: the Green function is required only on sites at this interface and for energies at the Fermi surface as $T \to 0$. The derivation of this formula is relatively simple and based on physical arguments.

This formula is proved to be equivalent to rigorous linear-response expressions for conductance coefficients. Its lower information requirements are particularly important for the efficiency when calculating the conductance by finite-difference approaches.

1. Introduction

The understanding of quantum phenomena revealed in mesoscopic physics has required a new formulation of transport properties, suitable to the phase-coherent regime. A particularly convenient formalism relates [1,2] the conductance coefficients to the transmission probabilities between the contacts. Recently, it has been rigorously demonstrated [3,4] that this formalism is equivalent to electrical linear-response theory, with the by-product of relations between the transmission amplitudes and the Green function of the system.

In this paper, starting from slightly different physical arguments, new conductance expressions for the mesoscopic regime are derived in a most direct way. The main result is a formula for the differential transmission current across an interface in terms of the Green function at the interface. It is a very general expression for independent-particle transport between two contiguous systems, owing much to the scanning tunnelling microscope theory presented in [5]. It is the starting point for retrieving the expression for the conductance coefficients of a multi-terminal device.

In section 2 the 'multi-branch' system is introduced, intended to be an extension of the multi-lead system. It is worth leaving the freedom for the branch to be other than a straight ordered lead, since the conductance coefficient does not depend on the specific modes but only involves Green functions. We can imagine more general semi-infinite branches for which we know the Green function.

In section 3 the expression for the differential current is derived, in the form of a two-terminal conductance. In section 4 it is shown how it can be generalized to multi-terminal conductance coefficients, simply by adapting the boundary conditions

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in order to let the current flow from one branch n to all other branches and retaining only the contribution to branch m, $m \neq n$.

Section 5 is devoted to a comparision with Baranger and Stone's rigorous expressions for the conductance in the linear-response approximation [4].

The conclusions contain some indications about the numerical implementation of the method.

2. Multi-branch system, Hamiltonian

The time independent tight binding Hamiltonian H describes a system of non-interacting spinless electrons with charge e, at $T = 0$, subject to an effective potential V and a magnetic field B characterized by the vector potential A. H is taken to be of the form

$$H = \sum_n |n\rangle H_{n,n} \langle n| + \sum_{n,n'} |n\rangle H_{n,n'} \langle n'| \tag{1}$$

where the first sum runs over all lattice sites and the second sum runs over all the ordered couples of nearest-neighbour lattice sites. (See for example [6] as a justification for the detailed form of such a Hamiltonian. For the purpose of this paper only the form of equation (1) matters.)

A finite central region (the probe) is joined by several branches to various chemical-potential reservoirs at infinity. The geometrical shape and Hamiltonian matrix elements of the probe are not subject to any constraints. It should be possible to determine the Green function of the isolated branches on some interface.

The chemical-potential reservoirs conform to the ones originally considered by Büttiker [2] in his model for a multi-terminal conductor. (i) They are large enough relative to the conductor, for any steady-state current flowing from or to them not to affect the constant value of their chemical potential, μ_l. (ii) No particle entering the reservoirs returns to the conductor without an inelastic event (and the reservoirs are indeed the only part of the system where phase-randomization does occur). (iii) Each branch reaches its reservoir in such an adiabatic way that the interface between them generates no additional resistance.

Büttiker [2] let the potentials μ_l be arbitrary within a narrow enough range at the Fermi energy, for the energy dependence of the transmission and reflection probabilities T_{mn} in this range to be negligible, and expressed the current coming out of each lead m (by means of the standard Landauer counting argument) as

$$I_m = \frac{e}{h}\left[(T_{mm} - N_m)\mu_m + \sum_{n \neq m} T_{mn}\mu_n\right] = \sum_n g_{mn} V_n \tag{2}$$

where the identity derived from current conservation $\sum_n T_{mn} - N_m = 0$ is in force. (Here N_l is the number of quantum channels in lead l. $T_{mn} = \sum_{ij} T_{mn,ij}$; $T_{mn,ij}$ denotes the probability of a carrier incident in lead n in channel j to be transmitted, or reflected if $m = n$, into lead m into channel i.)

Büttiker's multi-terminal Landauer formula (2) expresses the current response of a multi-terminal conductor in terms of applied external voltages on the leads, $V_l = \mu_l/e$. The crucial feature of Büttiker's approach is to treat the current and

voltage probes on equal footing: if a given set of injected currents is fixed instead, then the corresponding voltage response is found by appropriately inverting equation (2).

Baranger and Stone [4] rigorously derived the electrical linear current response of a multi-lead sample with applied constant voltages on the leads at frequency Ω in the limit of Ω going to zero. The phase-breaking mechanism was introduced via the infinite perfect leads, which in the linear-response model mimick well the boundary conditions of large phase-randomizing reservoirs. The scattering version of their results confirmed Büttiker's multi-terminal Landauer formula (2).

The multi-branch sample chosen here is explicitly attached to chemical potential reservoirs, allowing a rather physical derivation of the current picture. Putting one reservoir at an infinitesimally higher potential than the others one can deduce the boundary conditions, which consist of imposing only outgoing states in all other branches, and then express the transmission currents in terms of Green functions. The differential transmission currents, normalized by e^{-1}, therefore represent the differential conductance response of the sample, g_{mn} for $m \neq n$, when subject to an externally applied voltage configuration.

3. Two-branch conductance

Choose a finite interface dividing the system into a LHS part A and a RHS part B. Without loss of generality, the TB lattice is required to have no lattice sites on the interface. To calculate the differential conductance from A to B through the interface, the same procedure as in [5] is used, but extended to a non-symmetric Hamiltonian produced by the magnetic field.

Define

$$H^{(1)}_{\mathrm{A,B}} := \sum_{n\in\mathrm{A},\ n'\in\mathrm{B}} |n\rangle H_{n,n'}\langle n'| \tag{3}$$

$$H^{(1)} := H^{(1)}_{\mathrm{A,B}} + H^{(1)\,\dagger}_{\mathrm{A,B}} \tag{4}$$

$$H^{(0)} := H - H^{(1)}. \tag{5}$$

$H^{(0)}$ is the Hamiltonian corresponding to the systems A and B separated by a hard wall erected on the interface. P_M shall denote the projection operator on the lattice site set M; let I_{A} (I_{B}) be the set of lattice sites n (n'), contributing a non-vanishing amount to (3) (roughly speaking they are the TB interface on the A (on the B) side), see figure 1.

Eigenstates of $H^{(0)}$ confined by the hard wall to one side or other form a complete set. Those on the A side, $|\varphi^{(0)}_a\rangle$, are of the form,

$$P_{\mathrm{A}}|\varphi^{(0)}_a\rangle = |\varphi^{\mathrm{A}}_a\rangle \qquad P_{\mathrm{B}}|\varphi^{(0)}_a\rangle \equiv 0 \tag{6}$$

the set of $|\varphi^{\mathrm{A}}_a\rangle$ being a complete set of eigenfunctions of $P_{\mathrm{A}}H^{(0)}P_{\mathrm{A}}$ on A satisfying appropriate boundary conditions. $|\varphi^{(0)}_a\rangle$, corresponding to the hard wall in place, has no current sources on the B side, only at ∞ on the A side. When restoring the full

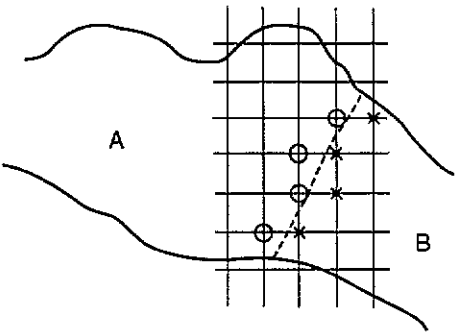

Figure 1. An arbitrary two-branch system. The dashed line indicates an interface I dividing it up into two semi-infinite subsystems A and B. No lattice sites are on I. The circled (crossed) lattice sites indicate the set $I_A(I_B)$, i.e. the lattice-site (TB) version of I on the A (B) side.

Hamiltonian, $H = H^{(0)} + H^{(1)}$, and removing the hard wall, the eigenstates $|\varphi_a^{(0)}\rangle$ of form (6) develop into eigenstates $|\varphi_a\rangle$ of H with the same energy ε_a,

$$|\varphi_a\rangle = (1 + G^{(0)}T)|\varphi_a^{(0)}\rangle$$

in particular

$$P_B|\varphi_a\rangle = G_B^{(0)}T_{BA}|\varphi_a^A\rangle. \tag{7}$$

Here the t-matrix is defined by

$$T = H^{(1)} + H^{(1)}GH^{(1)} \tag{8}$$

$$T_{BA} := P_B T P_A.$$

G and $G^{(0)}$ are the causal Green functions of H and $H^{(0)}$, and one can write

$$G^{(0)} = P_A G^{(0)} P_A + P_B G^{(0)} P_B =: G_A^{(0)} + G_B^{(0)}. \tag{9}$$

The trick of removing the barrier is going to be used to calculate the current flowing from A at Fermi energy $E_F + e\delta V$ to B at Fermi energy E_F: states $|\varphi_a^{(0)}\rangle$ have sources only in the reservoir at ∞ in A, and so do $|\varphi_a\rangle$, since removing the barrier introduces no new sources.

For the purpose of proof an infinitesimally small absorption mechanism is built into medium B, by adding on the B side an infinitesimal imaginary component, $-i\epsilon, \epsilon > 0$, to the energy. The idea is that the absorption taking place in B has to be balanced by the current flowing into B across the interface.

The time independent Schrödinger equation for an eigenstate $|\phi_E\rangle$ of the system $(A \cup B)$ reads, on the B side,

$$(E - i\epsilon)\phi = \frac{1}{2M}\left[\frac{\hbar}{i}\nabla - eA\right]^2 \phi + V\phi. \tag{10}$$

By multiplying equation (10) by ϕ^*, subtracting from the resulting equation its complex conjugate, and then integrating over B, one obtains

$$-2i\epsilon \int_B |\phi|^2 \, d^3r = -\int_{\partial B} \frac{i\hbar}{e} j_\phi \cdot n \, d^2S \tag{11}$$

with

$$j_\phi = \frac{e}{2M}\phi^*\left(\frac{\hbar}{\mathrm{i}}\nabla - eA\right)\phi + \frac{e}{2M}\phi\left(-\frac{\hbar}{\mathrm{i}}\nabla - eA\right)\phi^* \tag{12}$$

being the general expression for the electric current due to the state $|\phi\rangle$ in presence of local and electromagnetic potentials V, A and φ.

Here ∂B denotes the surface of B. For the states $|\varphi_a\rangle$ of the form (6), (7), contributions to the current from the surface at ∞ vanish because of absorption, so that an expression arises for the current transmitted from A to B due to the state $|\varphi_a\rangle$:

$$j_a^{\mathrm{T}} = -\int_{I_{\mathrm{B}}} j_{\varphi_a}\,\mathrm{d}^2S = -\int_{\partial\mathrm{B}} j_{\varphi_a}\,\mathrm{d}^2S = -\frac{2\epsilon e}{\hbar}\int_{\mathrm{B}}|\varphi_a|^2\,\mathrm{d}^3\mathbf{r}. \tag{13}$$

Now the current must be summed over all modes with energies between E_{F} and $E_{\mathrm{F}} + e\delta V$ so that the current δj^{T} from A to B induced by δV is

$$\delta j^{\mathrm{T}} = -\int_{\varepsilon_a\in[E_{\mathrm{F}},\ E_{\mathrm{F}}+e\delta V]}\mathrm{d}a\,\frac{2\epsilon e}{\hbar}\langle\varphi_a|P_{\mathrm{B}}|\varphi_a\rangle. \tag{14}$$

The differential conductance is then

$$g_{\mathrm{BA}}(E_{\mathrm{F}}) = \frac{\mathrm{d}j^{\mathrm{T}}}{\mathrm{d}V}(E_{\mathrm{F}}) = -\frac{2e^2\epsilon}{\hbar}\int \mathrm{d}a\,\langle\varphi_a^{\mathrm{A}}|T_{\mathrm{BA}}^\dagger G_{\mathrm{B}}^{(0)\dagger}G_{\mathrm{B}}^{(0)}T_{\mathrm{BA}}|\varphi_a^{\mathrm{A}}\rangle\delta(\varepsilon_a - E_{\mathrm{F}}). \tag{15}$$

Noticing that

$$\begin{aligned} G_{\mathrm{B}}^{(0)\dagger}G_{\mathrm{B}}^{(0)} &= \int \mathrm{d}b\int \mathrm{d}b'\,\frac{|\varphi_b^{\mathrm{B}}\rangle\langle\varphi_b^{\mathrm{B}}|\varphi_{b'}^{\mathrm{B}}\rangle\langle\varphi_{b'}^{\mathrm{B}}|}{(E-\varepsilon_b-\mathrm{i}\epsilon)(E-\varepsilon_{b'}+\mathrm{i}\epsilon)} \\ &= \frac{1}{2\mathrm{i}\epsilon}\int \mathrm{d}b\,|\varphi_b^{\mathrm{B}}\rangle\langle\varphi_b^{\mathrm{B}}|\left(\frac{1}{E-\varepsilon_b+\mathrm{i}\epsilon} - \frac{1}{E-\varepsilon_b-\mathrm{i}\epsilon}\right) \\ &= \frac{1}{2\mathrm{i}\epsilon}\left(G_{\mathrm{B}}^{(0)} - G_{\mathrm{B}}^{(0)\dagger}\right) \end{aligned} \tag{16}$$

and that

$$\begin{aligned} G_{\mathrm{A}}^{(0)} - G_{\mathrm{A}}^{(0)\dagger} &= \int \mathrm{d}a\,|\varphi_a^{\mathrm{A}}\rangle\langle\varphi_a^{\mathrm{A}}|\left(\frac{1}{E-\varepsilon_a+\mathrm{i}\epsilon} - \frac{1}{E-\varepsilon_a-\mathrm{i}\epsilon}\right) \\ &= \int \mathrm{d}a\,|\varphi_a^{\mathrm{A}}\rangle\langle\varphi_a^{\mathrm{A}}|2\mathrm{i}\,\mathrm{Im}\left(\frac{1}{E-\varepsilon_a+\mathrm{i}\epsilon}\right) \\ &= -2\mathrm{i}\pi\int \mathrm{d}a\,|\varphi_a^{\mathrm{A}}\rangle\langle\varphi_a^{\mathrm{A}}|\delta(E-\varepsilon_a) \end{aligned} \tag{17}$$

yields the expression

$$g_{\mathrm{BA}} = -\frac{e^2}{h}\,\mathrm{Tr}\left[T_{\mathrm{BA}}^\dagger\left(G_{\mathrm{B}}^{(0)} - G_{\mathrm{B}}^{(0)\dagger}\right)T_{\mathrm{BA}}\left(G_{\mathrm{A}}^{(0)} - G_{\mathrm{A}}^{(0)\dagger}\right)\right]. \tag{18}$$

Note that, due to the form of the Hamiltonian (1), the four implicit sums in this trace only run over the interface between A and B (two over I_{A} and two over I_{B}).

4. Multi-branch conductance coefficient

In an N_L-branch system, the conductance from branch n to branch $m \neq n$ is found in much the same way. Imagine reservoir n is at a chemical potential $E_F + e\delta V$ while all the others are at E_F, and erect $(N_L - 1)$ non-intersecting interfaces $J_l, l = 1, \ldots, N_L, l \neq n$, each one disconnecting from the system the corresponding branch l (subsystem S_l), and the whole of them leaving a subsystem connected with reservoir n, to be called $(S_n \cup D)$, D standing for the disordered part. $I := \bigcup_{l=1, l\neq n}^{N_L} J_l$ (see figure 2(*a*)).

Note, this prescription of how to choose the interface I is one among other possibilities. For example one could choose instead the partition of figure 2(*b*), which according to the circumstances could be more advantageous in practical calculations, where I is usually taken as short as possible.

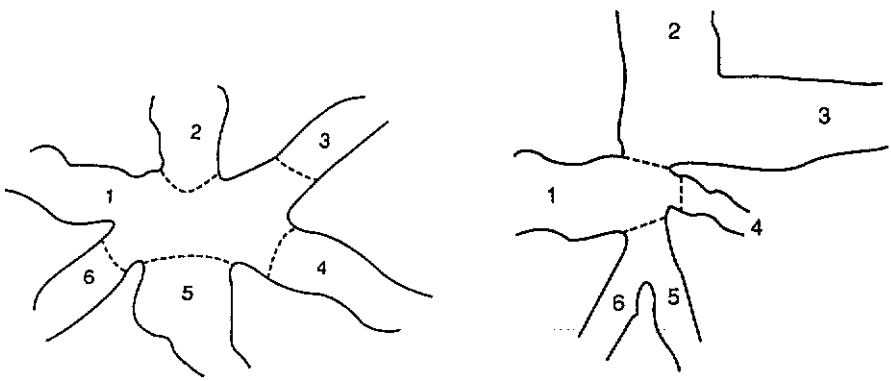

Figure 2. (*a*) Partition of a 6-branch system via interfaces J_l (dashed lines), $l = 2, \ldots, 6$, suitable for calculating the conductance coefficients $g_{m1}, m = 2, \ldots, 6$. (*b*) Possible alternative partition of a 6-branch system, suitable for calculating specifically the conductance coefficient g_{41} (as well as $(g_{21} + g_{31})$ and $(g_{51} + g_{61})$).

Again the interfaces are required to contain no lattice sites, to allow a unique definition of

$$H^{(1)}_{(S_n\cup D),\cup_{l\neq n} S_l} := \sum_{i\in(S_n\cup D), i'\in\cup_{l\neq n} S_l} |i\rangle H_{i,i'}\langle i'| \tag{19}$$

$$H^{(1)} := H^{(1)}_{(S_n\cup D),\cup_{l\neq n} S_l} + H^{(1)\dagger}_{(S_n\cup D),\cup_{l\neq n} S_l} \tag{20}$$

$$H^{(0)} := H - H^{(1)}. \tag{21}$$

$H^{(0)}$ is the Hamiltonian corresponding to the subsystems $(S_n \cup D)$ and $S_l, l = 1, \ldots, N_L, l \neq n$, separated by a hard wall erected on the interface I. The transmission current flowing from branch n to branch m through J_m is recognized to be the superposition of the states $|\varphi_a\rangle = (1 + G^{(0)}T)|\varphi_a^{(0)}\rangle$, for $|\varphi_a^{(0)}\rangle = P_{(S_n\cup D)}|\varphi_a^{(0)}\rangle = |\varphi_a\rangle^{(S_n\cup D)}$ (complete set on $(S_n \cup D)$) and $\varepsilon_a \in [E_F, E_F + e\delta V]$; and in branch m is built a fictitious absorption mechanism.

The corresponding differential conductance then is given by

$$g_{mn} = -\frac{e^2}{h}\,\mathrm{Tr}\left[T^{\dagger}_{S_m(S_n\cup D)}\left(G^{(0)}_{S_m} - G^{(0)\dagger}_{S_m}\right)T_{S_m(S_n\cup D)}\left(G^{(0)}_{(S_n\cup D)} - G^{(0)\dagger}_{(S_n\cup D)}\right)\right] \tag{22}$$

where T, G and $G^{(0)}$ refer to the Hamiltonians (1), (19)–(21), and low indices indicate on which subsystems these operators have been projected, as in the preceding section.

Again the four implicit sums in the trace only run over the interface I.

The hidden difference to the two-branch system, is that now I TB borders on the $(S_n \cup D)$ side the whole collection of interfaces $J_l, l = 1, \ldots, N_L, l \neq n$, and not just the interface J_m.

5. Comparision with Baranger and Stone's formalism

The purpose of this section is to compare expression (22) for the differential conductance coefficient to the one rigorously derived by Baranger and Stone [4] from linear-response theory. For this comparision the multi-branch system is restricted to a two-dimensional multi-lead probe (see figure 3(*a*)), which is the system considered in [4]: the branches are here straight, ordered leads. Ordered means in this context that the local potential is invariant under translations parallel to the lead. In each lead l, C_l denotes a cross section line located in the asymptotic region of lead l, where the electric field is zero. A local coordinate system (x_l, y_l) is defined, the x_l-axis being parallel to lead l and pointing to its asymptotical region (see figure 3(*b*)). Explicit use shall be made of the local coordinates belonging to the cross-section lines ; by convention, in each lead l, the origin of the x_l-axis is chosen so, that the equation $x_l = l + 1/2$ defines the cross-section line C_l. In the asymptotic region the magnetic field is required to be perpendicular to the leads and constant in each lead l.

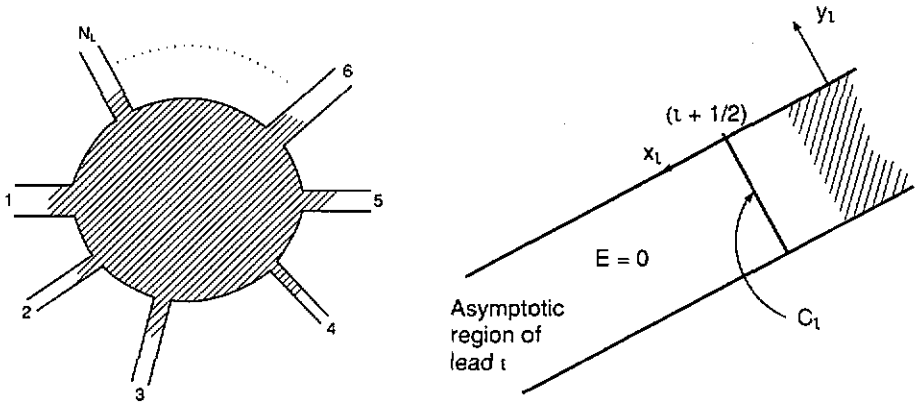

Figure 3. (*a*) An arbitrary multiprobe structure. A possibly disordered region (hatched) is connected to N_L straight, ordered leads which are used to feed current or measure voltage. (*b*) Asymptotic region of lead l. C_l is a cross-section line in lead l located in the asymptotic region (non-hatched) where the electric field is zero. A local coordinate system (x_l, y_l) is defined, the x_l-axis being parallel to lead l, pointing to its asymptotical region, and having the origin such that the equation $x_l = l + 1/2$ defines the cross-section line C_l.

Following [4], the conductance in scattering language involves eigenstates of the *infinite* perfect leads and transmission amplitudes between them, for energies near the Fermi level.

Given an infinite perfect lead l in a Landau gauge with translational symmetry in the x_l direction, its eigenstates can be written as (equations (55)–(58) in [4])

$$\xi_a^{\pm(l)}(x_l) = \frac{1}{\sqrt{\vartheta_a^{(l)}}} e^{\pm i k_a x} \chi_{j_a}^{\pm(l)}(y) \tag{23}$$

where $\vartheta_a^{(l)}$ is defined as the outgoing particle flux carried by $|\xi_a^{+(l)}\rangle$ through the lead cross section C_l, and the χs are normalized as

$$\sum_{y_l} |\chi_{j_a}^{\pm(l)}(y)|^2 = 1 \tag{24}$$

and satisfy the reduced transversal Schrödinger equation.

$t_{mn,ca}$ is defined as the transmission amplitude for going from mode a in lead n to mode c in lead m; the transmission amplitudes appear in the scattering-wave states as (equation (79) in [4])

$$\psi_{n,a}^{+}(x) \longrightarrow \xi_a^{-(n)}(x_n) + \sum_c^{\varepsilon} t_{nn,ca} \xi_c^{+(n)}(x_n) \qquad x \text{ in lead } n$$

$$\psi_{n,a}^{+}(x) \longrightarrow \sum_c^{\varepsilon} t_{mn,ca} \xi_c^{+(n)}(x_m) \qquad x \text{ in lead } m, m \neq n \tag{25}$$

where

$$\sum_a^{\varepsilon} := \int \mathrm{d}a\, \delta(\varepsilon - \varepsilon_a)$$

denotes a restricted sum over a at energy ε. Baranger and Stone's expression for the conductance coefficient from lead n to lead m is (equations (77), (89) and (B16) respectively, in [4])

$$g_{mn} = \frac{e^2\hbar}{2\pi} \int \mathrm{d}\varepsilon\, [-f'(\varepsilon)] \sum_{a,c}^{\varepsilon} |f_{mn,ca}^{\varepsilon}|^2 \qquad m \neq n \tag{26}$$

$$t_{mn,ca} = i\hbar f_{mn,ca}^{\varepsilon} \qquad m \neq n \tag{27}$$

$$t_{mn,ca} = -\frac{i\hbar}{e^2} \langle \xi_c^{+(m)} | K_{\mathrm{op}}(m) G_{\varepsilon} K_{\mathrm{op}}(n) | \xi_a^{-(n)} \rangle \qquad m \neq n. \tag{28}$$

Here G_{ε} is the causal Green function; $K_{\mathrm{op}}(l)$ refers to lead l and is a Hermitian operator which represents the current going through the bonds between the columns $x_l = l$ and $x_l = l + 1$:

$$K_{\mathrm{op}}(l) = \frac{e}{i\hbar} \sum_{l_y} (V_{l,l_y}^{x} |l, l_y\rangle\langle l+1, l_y| - V_{l,l_y}^{x*} |l+1, l_y\rangle\langle l, l_y|)$$

with

$$V_{l,l_y}^{x} = \langle l, l_y | H | l+1, l_y \rangle \tag{29}$$

where the sites are labeled by pairs of integers in the local coordinates (x_l, y_l).

For $T = 0$, g_{mn} only depends on the Fermi energy $\varepsilon = E_F$ as

$$g_{mn} = \frac{\hbar}{2\pi e^2}\sum_{a,c}^{\varepsilon} |\langle \xi_c^{+(m)}|K_{op}(m)G_\varepsilon K_{op}(n)|\xi_a^{-(n)}\rangle|^2. \tag{30}$$

Equation (30) can be rewritten as

$$g_{mn} = \frac{\hbar}{2\pi e^2}\sum_{a}^{\varepsilon}\langle \xi_a^{-(n)}|K_{op}(n)G_\varepsilon^\dagger K_{op}(m)\sum_{c}^{\varepsilon}|\xi_c^{+(m)}\rangle\langle\xi_c^{+(m)}|K_{op}(m) \times G_\varepsilon K_{op}(n)|\xi_a^{-(n)}\rangle \tag{31}$$

and simplified by proving that

$$K_{op}(m)\sum_{c}^{\varepsilon}|\xi_c^{+(m)}\rangle\langle\xi_c^{+(m)}|K_{op}(m) \propto K_{op}(m)$$

on the subspace of interest.

The asymptotic behaviour of G_ε and $G_\varepsilon^\dagger$ between different leads is (see equation (66) in [4] and the adjoint of it)

$$G_\varepsilon(x_m, x_n) = \sum_{a,c}^{\varepsilon} f_{mn,ca}^{\varepsilon}\xi_a^{+(m)}(x_m)\xi_c^{-(n)*}(x_n)$$

$$G_\varepsilon^\dagger(x_n, x_m) = \sum_{a,c}^{\varepsilon} f_{mn,ca}^{\varepsilon *}\xi_a^{+(m)*}(x_m)\xi_c^{-(n)}(x_n), (m \neq n). \tag{32}$$

The current conservation identity (equation (B11) in [4]),

$$\langle \xi_a^{\pm}|K_{op}(n)|\xi_{a'}^{\pm}\rangle = \pm e\delta_{aa'}$$

for $\varepsilon_a = \varepsilon_{a'}$ implies that for states all at the same energy ε:

$$\langle \xi_a^{+(m)}|K_{op}(m)\sum_{c}^{\varepsilon}|\xi_c^{+(m)}\rangle\langle\xi_c^{+(m)}|K_{op}(m)|\xi_{a'}^{+(m)}\rangle = e\langle\xi_a^{+(m)}|K_{op}(m)|\xi_{a'}^{+(m)}\rangle$$

so equation (31) simplifies to

$$g_{mn} = \frac{\hbar}{2\pi e}\sum_{a}^{\varepsilon}\langle \xi_a^{-(n)}|K_{op}(n)G_\varepsilon^\dagger K_{op}(m)G_\varepsilon K_{op}(n)|\xi_a^{-(n)}\rangle. \tag{33}$$

Now the equivalence will be shown between equations (33) and (22).

In each lead l, P_l shall denote the projection on $x_l = l$, P_{l+1} the projection on $x_l = l + 1$;

$$P_l V P_{l+1} := \sum_{l_y} V_{l,l_y}^{x}|l, l_y\rangle\langle l+1, l_y| \tag{34}$$

with the lattice sites in the local coordinates x_l,

$$P_{l+1}V^{\dagger}P_l := (P_lVP_{l+1})^{\dagger}. \tag{35}$$

$$H^{(1)}_{(S_n\cup D),\cup_{l\neq n}S_l} := \sum_{l,l\neq n} P_lVP_{l+1} \tag{36}$$

$$H^{(1)} := H^{(1)}_{(S_n\cup D),\cup_{l\neq n}S_l} + H^{(1)\dagger}_{(S_n\cup D),\cup_{l\neq n}S_l} \tag{37}$$

$$H^{(0)} := H - H^{(1)}. \tag{38}$$

$H^{(0)}$ corresponds to a system with hard walls on all the cross sections except on C_n. The partition of the multi-lead probe is fully analogous to that of the multi-branch system in the preceding section; for $l \neq n$, the previous interfaces J_l are now straight cross sections C_l. Using the same notation as before, S_m is the disconnected part of lead m, and $(S_n \cup D)$ is the subsystem connected to the reservoir n, D denoting the disordered part of the N_L-lead system limited by the cross sections. T and $G^{(0)}$ are labeled again according to their projections on the subsystems. In particular

$$T_{S_m(S_n\cup D)} = P_{S_m}TP_{(S_n\cup D)} = P_{m+1}(H^{(1)} + H^{(1)}GH^{(1)})\sum_{l\neq n}P_l. \tag{39}$$

Equation (33) then reads

$$\begin{aligned} g_{mn} &= -\frac{\mathrm{i}}{2\pi}\sum_a^e \{\langle\xi_a^{-(n)}|K_{\mathrm{op}}(n)G^{\dagger}P_mVP_{m+1}GK_{\mathrm{op}}(n)|\xi_a^{-(n)}\rangle \\ &\quad - \langle\xi_a^{-(n)}|K_{\mathrm{op}}(n)G^{\dagger}P_{m+1}V^{\dagger}P_mGK_{\mathrm{op}}(n)|\xi_a^{-(n)}\rangle\} \\ &= -\frac{\mathrm{i}}{2\pi}\sum_a^e \{\langle\xi_a^{-(n)}|K_{\mathrm{op}}(n)[G^{(0)\dagger}_{(S_n\cup D)} + G^{(0)\dagger}_{(S_n\cup D)}H^{(1)}G^{\dagger}]P_mVP_{m+1} \\ &\quad \times G^{(0)}_{S_m}T_{S_m(S_n\cup D)}G^{(0)}_{(S_n\cup D)}K_{\mathrm{op}}(n)|\xi_a^{-(n)}\rangle \\ &\quad - \langle\xi_a^{-(n)}|K_{\mathrm{op}}(n)G^{(0)\dagger}_{(S_n\cup D)}T^{\dagger}_{S_m(S_n\cup D)}G^{(0)\dagger}_{S_m}P_{m+1}V^{\dagger}P_m \\ &\quad \times [G^{(0)}_{(S_n\cup D)} + GH^{(1)}G^{(0)}_{(S_n\cup D)}]K_{\mathrm{op}}(n)|\xi_a^{-(n)}\rangle\}. \end{aligned} \tag{40}$$

From equations (34)–(37) and the fact that the cross sections C_l do not intersect each other, it is evident that $P_mVP_{m+1} = H^{(1)}P_{m+1}$, so that

$$[G^{(0)\dagger}_{(S_n\cup D)} + G^{(0)\dagger}_{(S_n\cup D)}H^{(1)}G^{\dagger}]P_mVP_{m+1} = G^{(0)\dagger}_{(S_n\cup D)}[H^{(1)} + H^{(1)}G^{\dagger}H^{(1)}]P_{m+1}.$$

To get rid of the operators $K_{\mathrm{op}}(n)$, it can be observed that

$$|\varphi_a\rangle := \left(P_{[n+1,\infty[} + \frac{\mathrm{i}\hbar}{e}G^{(0)}_{(S_n\cup D)}K_{\mathrm{op}}(n)\right)|\xi_a^{-(n)}\rangle$$

is the state that develops on $(S_n \cup D)$ from the eigenstate $|\xi_a^{-(n)}\rangle$ of an *infinite* straight, ordered lead n, by first cutting it at $x_n = (n + 1/2)$ and then attaching the $[n+1,\infty[$-part of it to D. This process is discussed in appendix A and schematically

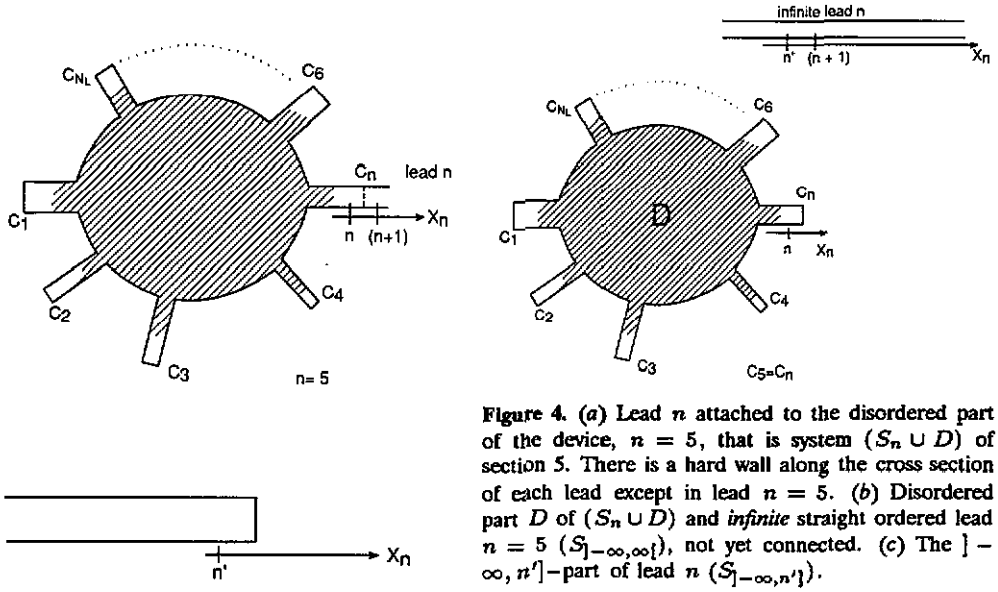

Figure 4. (*a*) Lead n attached to the disordered part of the device, $n = 5$, that is system $(S_n \cup D)$ of section 5. There is a hard wall along the cross section of each lead except in lead $n = 5$. (*b*) Disordered part D of $(S_n \cup D)$ and *infinite* straight ordered lead $n = 5$ $(S_{]-\infty,\infty[})$, not yet connected. (*c*) The $]-\infty, n']$–part of lead n $(S_{]-\infty,n'[})$.

consists of passing from the disconnected system in figure 4(*b*) to the disconnected system in figures 4(*a*) and 4(*c*) respectively.

Equation (40) then becomes

$$g_{mn} = -\frac{ie^2}{2\pi\hbar^2}\sum_a^{\epsilon} \langle\varphi_a|T^{\dagger}_{S_m(S_n\cup D)}\left(G^{(0)}_{S_m} - G^{(0)\dagger}_{S_m}\right)T_{S_m(S_n\cup D)}|\varphi_a\rangle.$$

This is now a sum over all the scattering-wave states at energy ϵ belonging to the subsystem $(S_n \cup D)$. The same algebra as displayed in equation (17) relates this sum to the unperturbed Green function on $(S_n \cup D)$. The determination of the normalization factor presents some subtleties, which are dealt with in appendix B. Equation (B5) expresses the correctly normalized relation. Making use of it, (41) finally turns into equation (22). This proves the equivalence between equations (33) and (22), which are in turn Baranger and Stone's conductance coefficients and the ones derived in this paper, for the discretized case and zero temperature.

Note, the differential conductance g^T_{mn} at an arbitrary temperature T can be expressed, in electrical linear response, as a Fermi-statistics weighted integral of $g^{T=0}_{mn}(E_F)$ over the whole continuum spectrum:

$$g^T_{mn} = \int d\varepsilon\,[-f'(\varepsilon)]g^{T=0}_{mn}(\varepsilon)$$

(see for example equation (77) in [4], which is reproduced here as equation (26)), so, with this method, the differential conductance at arbitrary temperature takes the form

$$g^T_{mn} = \int d\varepsilon\,[-f'(\varepsilon)]\left(-\frac{e^2}{h}\right)\mathrm{Tr}\left[\left(G^{(0)}_{(S_n\cup D)} - G^{(0)\dagger}_{(S_n\cup D)}\right)T^{\dagger}_{S_m(S_n\cup D)} \times \left(G^{(0)}_{S_m} - G^{(0)\dagger}_{S_m}\right)T_{S_m(S_n\cup D)}\right] \tag{41}$$

where of course the equivalence to [4] still holds.

In the frame of particle independence, while the formula (41) for an arbitrary T expresses the differential conductance in electrical linear response, its $(T = 0)$-version (see equation (22)) is an exact expression for the differential conductance, as can be verified by its derivation in sections 3 and 4.

6. Conclusions

A new useful expression for the conductance coefficients of multiprobe systems has been presented in discretized space: it is suited to the mesoscopic phase-coherent regime, within the independent-particle approximation. The derivation is transparent, based on physical arguments, and the agreement with analogous results from linear-response theory has been proved.

An important new aspect of this formula is that no specific assumptions are made on the asymptotic region of the terminals (called branches to stress their arbitrariness), except that they are connected to chemical potential reservoirs. Hence, on one hand, geometries other than multi-lead systems could become of interest and are treatable within this approach, provided that the Green function (GF) of each arbitrarily disconnected branch is known on the end surface. There is a consequence, on the other hand, relevant for the presently considered multi-lead systems, concerning the lattice site set on which GF knowledge is required: instead of lead cross sections the absence of asymptotic assumptions allows the interfaces to be chosen freely, as long as the required topology is respected. Numerical efficiency can only benefit from this flexibility.

A peculiarity of this conductance expression is that it involves, beside the t-matrix, the individual GFs belonging to different subsystems of the partitioned device. In usual algorithms, these individual GFs need to be calculated anyway to extract the t-matrix (or the full GF of the whole device, as is required by the conductance expression in [4]). Using these individual GFs explicitly in the conductance expression reduces, for few leads, the number of cross section columns on which GF knowledge is required (see [4] for a comparision). This gives rise to a further gain in computational efficiency.

For numerical applications, this conductance expression is naturally suited to be incorporated in finite-difference techniques (slab-by-slab linking [7] or particularly bond-by-bond linking [6]): starting with the GF elements at the end surface of an arbitrarily disconnected semi-infinite branch, the structure is grown, say bond-by-bond, and at each step the projection of the GF of the current cluster is known on the growing surface. Growth continues until hitting the interface (or collection of interfaces) of the chosen partition. The same procedure is repeated for each other branch. In the end this process supplies the GF elements entering the conductance expression, and needs no updating in addition to that required by the growth itself. Avoiding intermediate finite clusters spares GF singularities and confers a remarkable stability to the algorithm.

For the presently considered multi-lead systems, where each straight ordered lead is subject to a perpendicular constant magnetic field and a local, longitudinally invariant potential, the initial set of GF elements of a semi-infinite lead can be calculated following the elegant method described in [8].

Note, a tight-binding approach to multiprobe systems which also grows clusters starting from semi-infinite leads and obtains the conductance by means of various quantities, recursively updated only on the growing surface, is described in [9].

As examples of other branches which may become of interest and be treated with this method, could be mentioned a half plane under constant magnetic field connected via an arbitrary finite lead to the central part of the device, or a branch obtained by adiabatically widening a lead to a large region (which is the reservoir).

This conductance expression, incorporated in bond-by-bond finite-difference calculations [6], has been successfully tested for a wide collection of simple two-lead systems and for a four-lead system (a ballistic cross). Calculations on more complex and new systems are underway.

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Appendix A

This appendix relates to the multi-lead system of section 5. The system is not the original one, there are hard walls on each cross section C_l, for $l \neq n$. The subsystem $(S_n \cup D)$ consists of the lead n attached to the disordered part D, limited by these hard walls on the other leads. An expression is derived for the states that develop on $(S_n \cup D)$ from incoming eigenstates of the *infinite* straight ordered lead n, $S_{]-\infty,\infty[}$.

Start with the disordered part D and the *infinite* straight, ordered lead $S_{]-\infty,\infty[}$ not yet connected, where a hard wall on C_n, between $x_n = n$ and $x_n = (n+1)$, marks the boundary of D on lead n (see figure 4(*b*)).

At n' the coordinate x_n takes the value n, the prime indicates that it refers to sites on the infinite lead $S_{]-\infty,\infty[}$, whereas n refers to sites on D.

Let $H^{(0)} = H_D^{(0)} + H^{(0)}_{S_{]-\infty,\infty[}}$ be the Hamiltonian corresponding to the system of figure 4(*b*). The Hamiltonian $(H_{(S_n \cup D)} + H_{S_{]-\infty,n']}})$, corresponding to the two disconnected systems $(S_n \cup D)$ and $S_{]-\infty,n']}$ (see figures 4(*a*) and 4(*c*) respectively), is restored by acting on the system of figure 4(*b*) with the perturbing Hamiltonian

$$H^{(1)} = [-(P_{n'} V P_{n+1} + P_{n+1} V^\dagger P_{n'})] + [P_n V P_{n+1} + P_{n+1} V^\dagger P_n] \tag{A1}$$

where the first bracketed summand breaks the infinite $S_{]-\infty,\infty[}$ into the two semi-infinite $S_{]-\infty,n']}$ and $S_{[n+1,\infty[}$, and the second bracketed summand attaches $S_{[n+1,\infty[}$ to D. ($P_l V P_{l+1}$ and $P_{l+1} V^\dagger P_l$ contain the original Hamiltonian bonds across the cross section C_l, their definition was given in equations (34) and (35).)

$|\xi_a^{-(n)}\rangle$ (see equation (23)) is an eigenstate of $H^{(0)}_{S_{]-\infty,\infty[}}$ on the infinite lead and therefore an eigenstate of $H^{(0)}$. Under the action of $H^{(1)}$ it develops into an

eigenstate $|\psi_a\rangle$ of H, whose projection on $(S_n \cup D)$, $|\varphi_a\rangle := P_{(S_n \cup D)}|\psi_a\rangle$, is given by

$$|\varphi_a\rangle = P_{S_{[n+1,\infty[}}|\xi_a^{-(n)}\rangle + G_{(S_n \cup D)}(-P_{n+1}V^\dagger P_{n'} + P_n V P_{n+1})|\xi_a^{-(n)}\rangle$$
$$= (P_{S_{[n+1,\infty[}} + \frac{i\hbar}{e} G_{(S_n \cup D)} K_{op}(n))|\xi_a^{-(n)}\rangle. \tag{A2}$$

Appendix B

We consider in this appendix the multi-lead system. It has been partitioned into the subsystems $(S_n \cup D)$ and $S_l, l \neq n$, by erecting hard walls on the cross sections C_l for $l \neq n$. This partition is referred to as the unperturbed system as was done in section 5, with corresponding $H^{(0)}$ (defined in equations (36)–(38)) and $G^{(0)}$. Only the projection of $G^{(0)}$ on $(S_n \cup D)$, $G^{(0)}_{(S_n \cup D)}$, will be considered, and the purpose is to determine the normalization factor entering the relation between Green function and scattering-wave states at same energy on the subsystem $(S_n \cup D)$, to make the link between equations (41) and (22).

The causal Green function G of the full Hamiltonian H on the bare multi-lead system (without hard walls) must satisfy the same boundary conditions as the scattering-wave states in equation (25). Therefore $G^{(0)}_{(S_n \cup D)}$ satisfies the same boundary conditions as the incoming functions $|\xi_a^{-(n)}\rangle$ in lead n plus backscattered waves on $(S_n \cup D)$. The eigenfunctions of $H^{(0)}$ are either scattering-wave states of the form

$$|\varphi_a\rangle = (P_{S_{[n+1,\infty[}} + \frac{i\hbar}{e} G^{(0)}_{(S_n \cup D)} K_{op}(n))|\xi_a^{-(n)}\rangle \tag{B1}$$

(see appendix A) or bound states. Note $G^{(0)\dagger}_{bound} = G^{(0)}_{bound}$, hence

$$G^{(0)}_{(S_n \cup D)}(\varepsilon) - G^{(0)\dagger}_{(S_n \cup D)}(\varepsilon) = G^{(0)}_{(S_n \cup D)scatt}(\varepsilon) - G^{(0)\dagger}_{(S_n \cup D)scatt}(\varepsilon)$$
$$= -2i\pi \int da \frac{|\varphi_a\rangle\langle\varphi_a|}{N_a} \delta(\varepsilon - \varepsilon_a) \tag{B2}$$

(see equation (17)).

The normalizing factor N_a, can be determined by looking at the completeness relation of the set of eigenfunctions $|\xi_a^{\pm(n)}\rangle$ on an infinite lead:

$$1 = \int da \frac{\vartheta_a^{(n)}}{2\pi} (|\xi_a^{+(n)}\rangle\langle\xi_a^{+(n)}| + |\xi_a^{-(n)}\rangle\langle\xi_a^{-(n)}|)$$

from which

$$N_a = \frac{2\pi}{\vartheta_a^{(n)}}. \tag{B3}$$

We now make explicit the link between $\int da$ and

$$\sum_a^\varepsilon = \int da\, \delta(\varepsilon - \varepsilon_a)$$

for the scattering wave states of $H^{(0)}$ on $(S_n \cup D)$. In virtue of the one-to-one mapping relation (B1) it is sufficient to look at the dispersion relation of each channel in the infinite lead n.

$$\int \mathrm{d}a = \sum_j \int \mathrm{d}k = \sum_j \int \mathrm{d}\varepsilon_j \left(\frac{\partial \varepsilon_j}{\partial k}\right)^{-1} = \sum_j \int \mathrm{d}\varepsilon_j \frac{1}{\hbar v_{k,j}^{\|(n)}}$$
$$= \sum_j \int \mathrm{d}\varepsilon_j \frac{1}{(-\hbar \vartheta_{k,j}^{(n)})} = \int \mathrm{d}\varepsilon \sum_a^{\epsilon} \frac{1}{(-\hbar \vartheta_{k,j}^{(n)})} \qquad k = k(\varepsilon, j) \qquad \text{(B4)}$$

where $\vartheta_a^{(n)}$, defined as the outgoing particle flux carried by $|\xi_a^{+(n)}\rangle$, has been identified with the reversed longitudinal velocity,$(-v_a^{\|(n)})$, of $|\xi_a^{-(n)}\rangle$.

Finally gathering (B2),(B3) and (B4) yields the expression

$$G^{(0)}_{(S_n \cup D)}(\varepsilon) - G^{(0)\dagger}_{(S_n \cup D)}(\varepsilon) = \frac{\mathrm{i}}{\hbar} \sum_a^{\epsilon} |\varphi_a\rangle\langle\varphi_a|. \qquad \text{(B5)}$$

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