

Electronic transport at the nanoscale: the Non-Equilibrium Green's Function method

Rocco Martinazzo

Abstract

These notes focus on the main conceptual/theoretical steps needed to make the Non-Equilibrium Green's Function method suitable for investigating coherent ballistic transport on nanoscale devices or molecular junctions. The rich physics of the topic (e.g. the connection with different transport regimes, decoherence and dissipation, etc.) are well beyond the aim of these notes and is described in several textbooks.

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1 Green's operator (function)

The key quantity of interest is the following operator-valued function of the complex argument λ , known as *Green's* (or *resolvent*) *operator*

$$G(\lambda) = (\lambda - H)^{-1}$$

It is defined for any complex number for which $(\lambda - H)$ is not singular, *i.e.* the whole complex plane excluded the spectrum of H ; this (open) domain is also the region of *analyticity* of the function. As for any function of H , $G(\lambda)$ admits a spectral representation,

$$G(\lambda) = \int_{\sigma} \frac{1}{\lambda - E} p(E) d\mu(E)$$

where the differential eigenprojector $dP(E) := p(E)d\mu(E)$ is a standard projector for E a discrete eigenvalue (and the integral is just a sum), while for E in the continuous spectrum

$$dP(E) = \sum_i |E, i\rangle \langle E, i| dE$$

where $\{|E, i\rangle\}$ are improper eigenvectors at energy E and i is a degeneracy index. Formally, one can essentially identify $p(E)$ as a *density-of-states* operator¹, since the general expression

$$\delta(E - H) = \sum_n \delta(E - E_n) P_n + \chi_{\sigma_c}(E) \sum_i |E, i\rangle \langle E, i|$$

(where $\{E_n, P_n\}$ are the set of discrete eigenvalues/eigenprojectors, σ_c is the continuous spectrum and $\chi_A(E) = 1$ if $E \in A$, and $= 0$ otherwise) reduces to

$$\delta(E - H) = \sum_i |E, i\rangle \langle E, i| \equiv p(E)$$

when $E \in \sigma_c$, and allows one to re-write the spectral resolution as ordinary integral over the whole spectrum

$$G(\lambda) = \int_{\sigma} \frac{1}{\lambda - E} \delta(E - H) dE \equiv \int_{\sigma_c} \frac{1}{\lambda - E} \delta(E - H) dE + \sum_{\alpha} \frac{1}{\lambda - E_{\alpha}} P_{\alpha} \quad (1)$$

The interesting properties of $G(\lambda)$ are related to its analyticity, which extends above and below the real axes, where the continuous spectrum of H forms a branch cut of the function and the discrete eigenvalues are first-order poles. $G(\lambda)$ makes thus a jump when crossing the continuous spectrum, as can be seen by considering (see Fig.1)

¹More properly, $p(E) \equiv \delta_{\mu}(E - H)$ where δ_{μ} is the delta distribution on the measure μ . Hence, $p(E) = \delta(E - H)$ when E is an improper eigenvalue, $p(E_n) = P_n$ for E equal to the eigenvalue E_n and $P = 0$ otherwise.

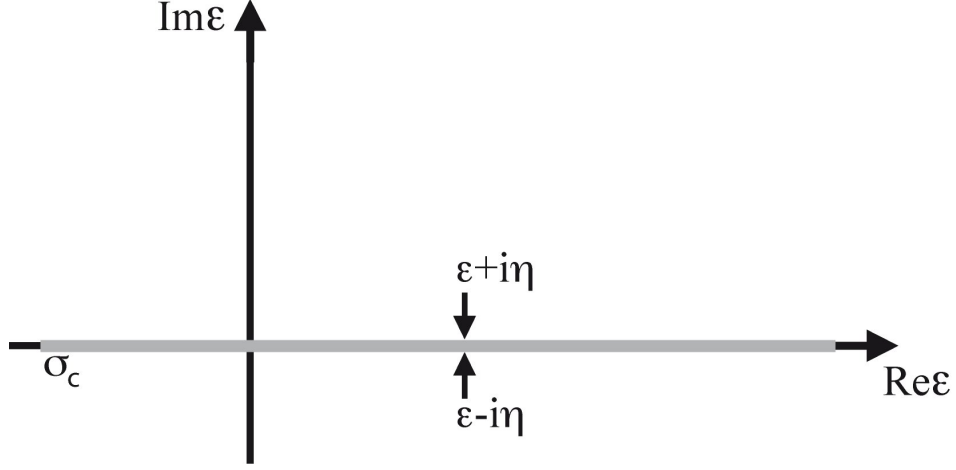


Figure 1: The limiting process on the complex energy plane described in the main text, here for $\lambda = \mathcal{E} \pm i\eta$.

$$\lim_{\epsilon \rightarrow 0^+} G(E \pm i\epsilon) = G^\pm(E) \quad (2)$$

for $E \in \sigma_c$. Indeed, upon using

$$\frac{1}{E + i\epsilon - E'} - \frac{1}{E - i\epsilon - E'} = \frac{(E - i\epsilon - E') - (E + i\epsilon - E')}{(E - E')^2 + \epsilon^2} = -\frac{2i\epsilon}{(E - E')^2 + \epsilon^2}$$

and taking the limit $\epsilon \rightarrow 0^+$ we obtain

$$G^+(E) - G^-(E) = -2\pi i \delta(E - H) \quad (3)$$

where

$$\delta(E - E') = \lim_{\epsilon \rightarrow 0^+} \frac{1}{\pi} \frac{\epsilon}{(E - E')^2 + \epsilon^2}$$

has been used. Since

$$G(\lambda)^\dagger = G(\lambda^*)$$

we also have

$$G^+(E)^\dagger = G^-(E)$$

and thus²

$$G^+(E) - G^-(E) = G^+(E) - G^+(E)^\dagger = 2i \text{Im} G^+(E)$$

i.e.

$$\text{Im} G^+(E) = -\pi \delta(E - H) \quad (4)$$

²The real and imaginary parts of an operator are defined with the help of the usual algebraic expressions, once the adjoint is recognized to be a conjugation operation. Namely, $\text{Re}A = (A + A^\dagger)/2$ and $\text{Im}A = (A - A^\dagger)/2i$.

On the other hand the real part of $G^+(E)$ is given by:

$$\begin{aligned} \operatorname{Re}G^+(E) &= \lim_{\epsilon \rightarrow 0^+} \int \operatorname{Re} \left[\frac{1}{E + i\epsilon - E'} \right] \delta(E' - H) dE' = \lim_{\epsilon \rightarrow 0^+} \int \frac{E - E'}{(E - E')^2 + \epsilon^2} \delta(E - H) dE' \\ &= \mathbb{P} \int \frac{1}{E - E'} \delta(E - H) dE' = G^p(E) \end{aligned}$$

where \mathbb{P} stands for the *principal value* of the integral:

$$\mathbb{P} \int \frac{f(E')}{E - E'} dE' = \lim_{\delta \rightarrow 0} \left\{ \int_{E' - \delta}^{E' + \delta} \frac{f(E')}{E - E'} dE' + \int_{E' + \delta} \frac{f(E')}{E - E'} dE' \right\}$$

Of course,

$$\operatorname{Re}G^-(E) = \operatorname{Re}G^+(E)$$

and thus³

$$G^\pm(E) = G^p(E) \mp i\pi\delta(E - H) \quad (5)$$

$G(\lambda)$ is connected to the evolution operator through analytic continuation of the appropriate Fourier-Laplace transform. Specifically, for $\operatorname{Im}\lambda > 0$ the integral

$$\int_0^{+\infty} e^{i\lambda t} e^{-iHt} dt$$

is well defined (convergent)⁴ and reads as

$$\int_0^{+\infty} e^{i\lambda t} e^{-iHt} dt = \int_0^{+\infty} e^{i(\lambda - H)t} dt = -iG(\lambda) e^{i(\lambda - H)t} \Big|_0^{+\infty} = iG(\lambda)$$

With the same token

$$-iG(\lambda)^\dagger = \int_0^{+\infty} e^{i\lambda^* t} e^{-iHt} dt = \int_{-\infty}^0 e^{-i\lambda^* t'} e^{iHt'} dt' = -iG(\lambda^*)$$

³This equation actually holds for any $E \in \mathbb{R}$. However, differently from what happens in the continuous spectrum, in the neighborhoods of a discrete eigenvalue E_n the r.h.s. is singular, being a true delta-like function, $\delta(E - E_n)P_n$ (see Eq.1). Thus, if $E \in \mathbb{R}/\sigma$ the imaginary part vanishes and $G^+(E) = G^-(E) = G^p(E)$. On the other hand, when the limit is taken (from any direction) to $E = E_n$ the function $G(\lambda)$ diverges as $(E - E_n)^{-1}P_n$.

⁴For large t the integrand goes as $e^{i\lambda t} e^{-iHt} \propto e^{i(\operatorname{Im}\lambda)t} = e^{-\operatorname{Im}\lambda t}$, i.e. it decays exponentially to zero, the faster the larger $\operatorname{Im}\lambda$ is.

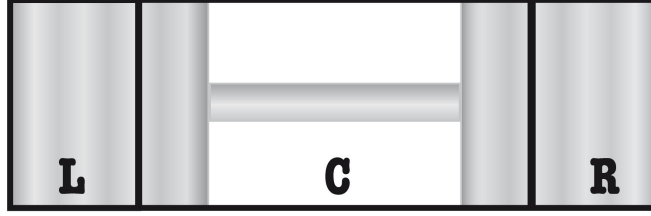


Figure 2: Setup for a two-terminal junction. L, R are the left and right electrodes, respectively, and C is the “conductor”.

where now λ^* lies in the lower half plane. Hence

$$G(\lambda) = -i \int_0^{+\infty} e^{i\lambda t} e^{-iHt} dt \quad \lambda \in \mathbb{C}^+$$

$$G(\lambda) = +i \int_{-\infty}^0 e^{i\lambda t} e^{-iHt} dt \quad \lambda \in \mathbb{C}^-$$

In particular,

$$G^+(E) = -i \lim_{\epsilon \rightarrow 0^+} \int_0^{+\infty} e^{iEt} e^{-iHt} e^{-\epsilon t} dt$$

$$G^-(E) = +i \lim_{\epsilon \rightarrow 0^+} \int_{-\infty}^0 e^{iEt} e^{-iHt} e^{\epsilon t} dt$$

or, equivalently, with the help of the Heavisid function $\Theta(t) = 1$ for $t > 0$ and $= 0$ otherwise,

$$G^\pm(E) = \mp i \lim_{\epsilon \rightarrow 0^+} \int_{-\infty}^{+\infty} \Theta(\pm t) e^{i(E-H)t} e^{-\epsilon|t|} dt$$

and we obtain the previous result

$$G^+(E) - G^-(E) = -i \int_{-\infty}^{+\infty} e^{i(E-H)t} dt = -2\pi i \delta(E - H)$$

These properties establish a connection between the energy eigenstates and the dynamics, making thus G suitable for describing transport across a nanostructure.

2 Green's operator for the (coupled) scattering region

We are interested in the setup of Fig. 2 where a *left electrode* L is connected to a *right electrode* R through a scattering region, the *conductor* C . L and R are infinite regions, but where electronic motion is non-interesting provided it does not interfere with the motion in C . We thus seek to express the relevant quantities in terms of operators pertaining to region C only. To this end, we first introduce the projection operators for the three regions, which satisfy

$$\begin{aligned} R^2 = R = R^\dagger \quad C^2 = C = C^\dagger \quad L^2 = L = L^\dagger \\ RL = LC = RC = 0 \quad R + L + C = 1 \end{aligned}$$

and consider

$$(\lambda - H)G(\lambda) = 1$$

in terms of the components in the above spaces. In doing this, we assume that C is large enough that $LHR = RHL = 0$, thereby obtaining

$$\begin{bmatrix} \lambda - H_{LL} & -H_{LS} & 0 \\ -H_{CL} & \lambda - H_{CC} & -H_{CR} \\ 0 & -H_{RC} & \lambda - H_{RR} \end{bmatrix} \begin{bmatrix} G_{LL}(\lambda) & G_{LC}(\lambda) & G_{LR}(\lambda) \\ G_{CL}(\lambda) & G_{CC}(\lambda) & G_{CR}(\lambda) \\ G_{RL}(\lambda) & G_{RC}(\lambda) & G_{RR}(\lambda) \end{bmatrix} = \begin{bmatrix} L & 0 & 0 \\ 0 & C & 0 \\ 0 & 0 & R \end{bmatrix}$$

We are interested in the middle-column equation only

$$\begin{cases} (\lambda - H_{LL})G_{LC}(\lambda) - H_{LC}G_{CC}(\lambda) = 0 \\ (\lambda - H_{CC})G_{CC}(\lambda) - H_{CL}G_{LC}(\lambda) - H_{CR}G_{RC}(\lambda) = 0 \\ (\lambda - H_{RR})G_{RC}(\lambda) - H_{RC}G_{CC}(\lambda) = 0 \end{cases}$$

Solving for G_{LC} and G_{RC} the first and the third equation,

$$G_{LC}(\lambda) = +g_L(\lambda)H_{CL}G_{CC}(\lambda)$$

$$G_{RC}(\lambda) = +g_R(\lambda)H_{RC}G_{CC}(\lambda)$$

where $g_L(\lambda)$ and $g_R(\lambda)$ are the Green's functions for the *uncoupled* left and right electrodes

$$g_L(\lambda) = (\lambda - H_{LL})^{-1} \quad \text{and} \quad g_R(\lambda) = (\lambda - H_{RR})^{-1},$$

we arrive at

$$[(\lambda - H_{CC}) - H_{CL}g_L(\lambda)H_{LC} - H_{CR}g_R(\lambda)H_{RC}]G_{CC}(\lambda) = C$$

Thus, the CC projection of the *exact* Green's function is the Green's function of an *effective Hamiltonian* in C space:

$$(\lambda - H_{eff}(\lambda))G_{CC}(\lambda) = C \tag{6}$$

where

$$H_{eff}(\lambda) = H_{CC} + H_{CL}g_L(\lambda)H_{LC} + H_{CR}g_R(\lambda)H_{RC}$$

In particular, for $\lambda = E + i\epsilon$, $\epsilon \rightarrow 0^+$, we write

$$H_{eff}(E) = H_{CC} + \Sigma_L^+(E) + \Sigma_R^+(E) \quad (7)$$

where

$$\Sigma_L^+(E) = H_{CL}g_L^+(E)H_{LC}$$

$$\Sigma_R^+(E) = H_{CR}g_R^+(E)H_{RC}$$

are the left and right so-called *self-energies* of the electrodes. They play the role of traditional energy-dependent *optical potentials* known in quantum scattering theory.

The self-energies have both a real and an imaginary part, which readily follows from the real and imaginary part of g_L^+ and g_R^+ , namely

$$\text{Re}\Sigma_L^+(E) = H_{CL}g_L^p(E)H_{LC} := \Delta_L(E)$$

$$\text{Im}\Sigma_L^+(E) = H_{CL}(-\pi\delta(E - H_{LL}))H_{LC} := -\frac{\Gamma_L(E)}{2}$$

With these definitions we can re-write the effective Hamiltonian as

$$H_{eff}(E) = H_{CC} + \Delta(E) - i\frac{\Gamma(E)}{2} \quad (8)$$

with

$$\Delta(E) = \Delta_L(E) + \Delta_R(E)$$

and

$$\Gamma(E) = \Gamma_L(E) + \Gamma_R(E)$$

both self-adjoint operators.

Note that for any state in C it holds a positivity condition⁵

$$\langle \phi_C | \Gamma_L(E) | \phi_C \rangle = 2\pi \langle \phi_C | H_{CL} \delta(E - H_{LL}) H_{LC} | \phi_C \rangle = 2\pi \langle H_{LC} \phi_C | \delta(E - H_{LL}) | H_{LC} \phi_C \rangle \geq 0$$

which means that Γ is a semi-positive defined operator,

$$\Gamma_{L,R}(E) \geq 0$$

The problem of determining $G_{CC}^+(E)$ thus reduces to the problem of computing the electrodes self-energies and build up (and invert) the effective Hamiltonian. It is obvious that the self-energies account for the motion in the regions L , R in which we are not interested. Note, however, that g_L (g_R) refers to H_{LL} (H_{RR}) *i.e.* to the dynamics in electrode L (R) when it is *not* coupled to the scattering region (otherwise we would need of G_{LL} instead of g_L).



Figure 3: Schematics for the iterative solution of the uncoupled left electrode Green's function.

3 Green's operators for the uncoupled electrodes

The left (right) electrode regions are infinite themselves, and no real simplification would occur if we could not compute the Green's operators

$$g_L^+(E) = (E^+ - H_{LL})^{-1}$$

Fortunately, in the self-energy expression

$$\Sigma_L^+(E) = H_{CL}g_L^+(E)H_{LC}$$

we only need those matrix elements $\langle \lambda | g_L^+(E) | \lambda' \rangle$ involving states $|\lambda\rangle, |\lambda'\rangle$ in L which *couple* to states in C , *i.e.* for which $\langle \lambda | H_{LC} | \phi_C \rangle \neq 0$. This is the key observation, which considerably simplifies the problem since reduces the potentially infinite states in the electrode to just “a few”.

Suppose then that H_{LC} is of “short” range and consider the region L_1 of L which couples to C *via* H_{CL} . L_2, L_3, \dots are regions of similar size which make up the remainder of the electrode's space, see Fig.3. As before we could use the partitioning technique and solve for $g_{11}(\lambda)$, the L_1L_1 projection of the exact Green's function on the uncoupled electrode, in terms of the self-energy of the remainder, $\Sigma_1^+(\lambda)$. In turn, we would need the self-energies $\Sigma_2^+(\lambda), \Sigma_3^+(\lambda), \dots, \Sigma_n^+(\lambda)$ (here the n -th term describes the motion in the uncoupled $L_{n+1} + L_{n+2} + \dots$ region) up to some high order N where we can reasonably truncate the procedure.

Alternatively, we consider $L_1, L_2 \dots$ large enough to interact with the nearest neighbors only, and write down the equation for $g_{11}(\lambda)$

$$\begin{bmatrix} \lambda - H_{11} & -V_{12} & 0 & 0 & 0 & 0 \\ -V_{21} & \lambda - H_{11} & -V_{23} & 0 & 0 & 0 \\ 0 & -V_{32} & \lambda - H_{11} & \dots & 0 & 0 \\ 0 & 0 & \dots & \dots & -V_{N-1N} & 0 \\ 0 & 0 & 0 & -V_{NN-1} & \lambda - H_{NN} & \dots \\ & & & & \dots & \dots \end{bmatrix} \begin{bmatrix} g_{11}(\lambda) \\ g_{21}(\lambda) \\ g_{31}(\lambda) \\ \vdots \\ g_{N1}(\lambda) \\ \dots \end{bmatrix} = \begin{bmatrix} L_1 \\ 0 \\ 0 \\ \vdots \\ 0 \\ \dots \end{bmatrix}$$

⁵More explicitly, introducing the electrode eigenvectors $|Ei, L\rangle, \langle \phi_C | \Gamma_L(E) | \phi_C \rangle = 2\pi \sum_i \langle \phi_C | H_{CL} | Ei, L \rangle \langle Ei, L | H_{LC} | \phi_C \rangle = 2\pi \sum_i |\langle Ei, L | H_{LC} | \phi_C \rangle|^2 \geq 0$

Upon truncating at the N -th order, the N -th equation reads as

$$-V_{NN-1}g_{N-1,1}(\lambda) + (\lambda - H_{NN})g_{N1}(\lambda) = 0$$

and can be solved for $g_{N,1}$,

$$g_{N1}(\lambda) = (\lambda - H_{NN})^{-1}V_{NN-1}g_{N-1,1}(\lambda)$$

Inserting this expression in the $N - 1$ -th equation we get rid of $g_{N,1}$

$$-V_{N-2,1}g_{N-2,1}(\lambda) + [\lambda - (H_{N-1,N-1} - V_{N-1,N}(\lambda - H_{NN})^{-1}V_{N,N-1})]g_{N-1,1} = 0$$

and obtain $g_{N-1,1}$

$$g_{N-1,1}(\lambda) = [\lambda - (H_{N-1,N-1} - V_{N-1,N}(\lambda - H_{NN})^{-1}V_{N,N-1})]^{-1}V_{N-2,1}g_{N-2,1}(\lambda)$$

which can be used similarly to above to eliminate $g_{N-1,1}$.

Keeping reasoning in this way, we arrive at

$$g_{11}(\lambda) = (\lambda - H_1^{eff}(\lambda))^{-1}L_1 \quad (9)$$

where

$$\begin{aligned} H_n^{eff}(\lambda) &= H_{nn} + \Sigma_n(\lambda) \\ \Sigma_n(\lambda) &= V_{nn+1}(\lambda - H_{n+1}^{eff}(\lambda))^{-1}V_{n+1n} \end{aligned} \quad \text{for } n = 1, 2, \dots \quad (10)$$

Truncation occurs when setting $V_{NN+1} = 0$, or equivalently $H_N^{eff} \cong H_{NN}$.

The above algorithm is completely general, and considerable simplifications occur when L_n are periodic images of each other. Indeed in this case, upon introducing the matrices \mathbf{H} and \mathbf{V} according to

$$\begin{aligned} \mathbf{H}_{nm} &= \langle \chi_n^{(1)} | H | \chi_m^{(1)} \rangle \\ \mathbf{V}_{nm} &= \langle \chi_n^{(1)} | V | \chi_m^{(2)} \rangle \end{aligned}$$

where $|\chi_m^{(1)}\rangle$ are basis vectors in cell 1 and $|\chi_m^{(2)}\rangle = T_{\mathbf{a}}|\chi_m^{(1)}\rangle$ are their periodic images ($T_{\mathbf{a}}$ is the corresponding translation operator), one obtains the Green's functions of interest

$$\mathbf{g}_{nm}(\lambda) = \langle \chi_n^{(1)} | g_L(\lambda) | \chi_m^{(1)} \rangle$$

upon solving the exact algebraic equation

$$\left[\lambda - (\mathbf{H} + \mathbf{V}\mathbf{g}(\lambda)\mathbf{V}^\dagger) \right] \mathbf{g}(\lambda) = \mathbf{1}$$

which is free of truncation errors.

4 Scattering states

The Green's function introduced above is the key-quantity for investigating transport across the conductor. In fact, it easily allows the determination of the scattering states, *i.e.* of those (improper) eigenvectors of the Hamiltonian which describe the evolution of a “free” propagating state into (and out) of the scattering region, as we now show.

According to the general scattering theory, the eigenstate $|Ei, L+\rangle$ which evolves from the freely propagating state $|Ei, L\rangle$ in the left electrode can be obtained as the limiting vector which solves the equation

$$(\lambda - H) |\psi_\lambda\rangle = (\lambda - H_{LL}) |Ei, L\rangle \quad (11)$$

when $\lambda = E + i\epsilon$, $\epsilon \rightarrow 0^+$. Notice that the above equation is well-defined and has a single solution for $\text{Im}\lambda \neq 0$, since $G(\lambda) = (\lambda - H)^{-1}$ exists above and below the real axis,

$$|\psi_\lambda\rangle = G(\lambda)(\lambda - H + H - H_{LL}) |Ei, L\rangle = [1 + G(\lambda)(H - H_{LL})] |Ei, L\rangle$$

i.e.

$$|Ei, L+\rangle = |Ei, L\rangle + G^+(E)(H - H_{LL}) |Ei, L\rangle$$

The advantage of using the above limiting process in defining the eigenstate $|Ei, L+\rangle$ (as opposite of the solution of the eigenvalue equation) is that one explicitly introduces in that way the desired boundary condition, namely $|Ei, L+\rangle \rightarrow |Ei, L\rangle$ when the interaction $H - H_{LL}$ is switched off.

In the above expression

$$L |Ei, L\rangle = |Ei, L\rangle$$

$$(H - H_{LL}) |Ei, L\rangle = H_{CL} |Ei, L\rangle$$

since $H_{RL} = 0$, hence

$$|Ei, L+\rangle = |Ei, L\rangle + G^+(E)H_{CL} |Ei, L\rangle$$

from which the components of $|Ei, L+\rangle$ in the R , C , and L spaces read as

$$|\phi_R\rangle := R |Ei, L+\rangle = G_{RC}^+(E)H_{CL} |Ei, L\rangle$$

$$|\phi_C\rangle := C |Ei, L+\rangle = G_{CC}^+(E)H_{CL} |Ei, L\rangle$$

$$|\phi_L\rangle := L |Ei, L+\rangle = |Ei, L\rangle + G_{LC}^+(E)H_{CL} |Ei, L\rangle$$

The latter in particular contains both an “incident” ($|Ei, L\rangle$) and a “scattered” term (second term on the r.h.s.).

Introducing the previously obtained expressions for the Green's function in the scattering region we obtain

$$|\phi_R\rangle = g_R^+(E)H_{RC}G_{CC}^+(E)H_{CL} |Ei, L\rangle \quad (12)$$

$$|\phi_C\rangle = G_{CC}^+(E)H_{CL} |Ei, L\rangle \quad (13)$$

$$|\phi_L\rangle = |Ei, L\rangle + g_L^+(E)H_{LC}G_{CC}^+(E)H_{CL}|Ei, L\rangle \quad (14)$$

now in terms of the fundamental G_{CC}^+ Green's function,

$$G_{CC}^+(E) = \lim_{\epsilon \rightarrow 0^+} \left(E + i\epsilon - H^{eff}(E) \right)^{-1} C$$

$$H^{eff}(E) = H_{CC} + \Sigma_R(E) + \Sigma_L(E)$$

$$\Sigma_L^+(E) = H_{CL}g_L^+(E)H_{LC}$$

$$\Sigma_R^+(E) = H_{CR}g_R^+(E)H_{RC}$$

It is obvious that, by construction, the vectors $|Ei, L+\rangle$ are eigenvectors of the full Hamiltonian with energy E . It can also be verified by an explicit calculation

$$\begin{aligned} (E - H)|Ei, L+\rangle &= (E - H)|Ei, L\rangle + (E - H)G^+(E)|Ei, L\rangle \\ &= (E - H_{CL} - H_{LL})|Ei, L\rangle = -H_{CL}|Ei, L\rangle + H_{CL}|Ei, L\rangle = 0 \end{aligned}$$

where $\lim_{\epsilon \rightarrow 0^+} (E - H)G^+(E) = 1$ and $(E - H_{LL})|Ei, L\rangle$ have been used.

The vectors $|Ei, L+\rangle$ contain the basic information we need to describe the scattering process. They play the same role that ordinary eigenvector play in bound state problems and can be obtained through Eq.s 12-14, from $G_{CC}(E)$.

Computation of $G_{CC}(E)$ amounts to invert the operator $(E - H^{eff})$ built with the effective Hamiltonian H^{eff} , for each (real) energy E of interest. H^{eff} is no longer self-adjoint, its eigenvalues are generally complex and its eigenvectors not orthogonal, and this raises the question of whether a spectral representation can be written for such an operator. In the finite-dimensional case, if the operator is diagonalizable, one finds the eigenvalues E_i , the eigenvectors $|i\rangle$ and their dual elements $\langle \bar{i}|$ defined by the condition⁶ $\langle \bar{i}|j\rangle = \delta_{ij}$, and then writes down

$$G_{CC}(\lambda) = \sum_i \frac{|i\rangle \langle \bar{i}|}{\lambda - E_i}$$

Equations 12-14 then determine the projection of the scattering states onto the R , C and L regions.

5 Self-consistency

So far we have assumed that the Hamiltonian is given and focused on how to express the quantities of interest in terms of the Green's function of the scattering region only. However

⁶If $|i\rangle$ is eigenvector of H^{eff} with eigenvalue E_i then the vector $|\bar{i}\rangle$ must be eigenvector of $(H^{eff})^\dagger$ with eigenvalue E_i^* . Indeed, if H^{eff} is diagonalizable there exists a set of eigenvectors spanning the whole space and the identity operator can be written as $1 = \sum_j |j\rangle \langle \bar{j}|$. Using this completeness relation we can write $\langle \bar{i}|H^{eff} = \sum_j \langle \bar{i}|H^{eff}|j\rangle \langle \bar{j}| = \sum_j E_j \delta_{ij} \langle \bar{j}| = E_i \langle \bar{i}|$, and take the adjoint of this expression.

H is at most a mean field Hamiltonian, *i.e.* an effective mono-electronic operator which has to be *self-consistent* with its solutions.

Consider first the equilibrium situation, where the same *chemical potential* μ applies to the R , L and C regions ($\mu_R = \mu_L = \mu_C = \mu$). The equilibrium condition is easily established by looking at the density of states and populating them up to the Fermi level (chemical potential). In other words, the one-electron density matrix (operator) γ of the central region C has to read as

$$\gamma = \int dE \delta(E - H^{eff}) f^\beta(E - \mu)$$

where $f^\beta(\mathcal{E})$ is the Fermi-Dirac distribution

$$f^\beta(\mathcal{E}) = \frac{1}{1 + e^{\beta\mathcal{E}}}$$

and $\delta(E - H^{eff})$ is the density-of-states operator of the scattering region. Then, according to Eq.4,

$$\gamma = -\frac{1}{\pi} \text{Im} \int_{-\infty}^{+\infty} G_{CC}^+(E) f^\beta(E - \mu) dE$$

which is usually evaluated by exploiting the analytic properties of $G_{CC}(\lambda)$ (along with the meromorphic character of $f^\beta(\mathcal{E})$), namely by replacing the path along the real axis with an equivalent path on the upper half plane, where $G_{CC}(\lambda)$ is free of singularities. Notice that μ is fixed by the normalization condition

$$\text{Tr}\gamma = N$$

where N is the number of electrons in the scattering region, what amounts to assume that polarization of charges occurs *within* the scattering region.

We can explicitly write the density-of-states operator in terms of the effective Hamiltonian H^{eff} by using

$$\begin{aligned} \text{Im}G_{CC}(\lambda) &= \text{Im} \left[G_{CC}(\lambda)(\lambda^* - H^{eff\dagger})G_{CC}^\dagger(\lambda) \right] = \\ &= G_{CC}(\lambda)\text{Im} \left(\lambda^* - H^{eff\dagger} \right) G_{CC}^\dagger(\lambda) = G_{CC}(\lambda) \left(\text{Im}\lambda^* - \frac{\Gamma(\lambda)}{2} \right) G_{CC}^\dagger(\lambda) \end{aligned}$$

and taking the limit⁷ $\lambda = E + i\epsilon$, $\epsilon \rightarrow 0^+$

$$\delta(E - H^{eff}) = \frac{1}{2\pi} G_{CC}^+(E)\Gamma(E)G_{CC}^-(E)$$

Taking into account that Γ has contributions from both the left and right electrodes, we end up with

$$\gamma = \gamma_L + \gamma_R$$

⁷Note that if Γ vanishes (*e.g.* for an isolated conductor) $\text{Im}\lambda^*$ cannot be neglected and the equation reads $\delta(E - H) = \frac{1}{\pi} \lim_{\epsilon \rightarrow 0^+} \epsilon G_{CC}(E + i\epsilon)G_{CC}(E - i\epsilon)$, see also the Note at the end of this document.

where

$$\gamma_L = \frac{1}{2\pi} \int dE f^\beta(E-\mu) G_{CC}^+(E) \Gamma_L(E) G_{CC}^-(E) = \int dE f^\beta(E-\mu) G_{CC}^+(E) H_{CL} \delta(E-H_{LL}) H_{LC} G_{CC}^-(E)$$

and similarly for R . In particular, the charge density at \mathbf{x} in the scattering region reads as

$$\rho(\mathbf{x}) = \rho_L(\mathbf{x}) + \rho_R(\mathbf{x})$$

where

$$\rho_L(\mathbf{x}) = \int dE f^\beta(E-\mu) \langle \mathbf{x} | G_{CC}^+(E) H_{CL} \delta(E-H_{LL}) H_{LC} G_{CC}^-(E) | \mathbf{x} \rangle$$

is the contribution of electrons from the left electrode and similarly for $\rho_R(\mathbf{x})$.

More precisely, with the help of the scattering states introduced above we can write down the contribution of the states which evolved from the left electrode

$$\begin{aligned} \delta_L(E-H^{eff}) &:= \sum_i C |Ei, L+\rangle \langle Ei, L+| C = \sum_i G_{CC}^+(E) H_{CL} |Ei, L\rangle \langle Ei, L| H_{LC} G_{CC}^-(E) = \\ &\equiv G_{CC}^+(E) H_{CL} \delta(E-H_{LL}) H_{LC} G_{CC}^-(E) \end{aligned}$$

and similarly for the right electrode and $\delta_R(E-H^{eff})$, or equivalently,

$$\delta_L(E-H^{eff}) = \frac{1}{2\pi} G_{CC}^+(E) \Gamma_L(E) G_{CC}^-(E), \quad \delta_R(E-H^{eff}) = \frac{1}{2\pi} G_{CC}^+(E) \Gamma_R(E) G_{CC}^-(E) \quad (15)$$

This observation is crucial to investigate the case where the system is in a *non-equilibrium* state, *i.e.* $\mu_R - \mu_L = \Delta\mu \neq 0$. In this case, indeed, it is reasonable to define the non-equilibrium density matrix as

$$\begin{aligned} \gamma &= \gamma_L + \gamma_R \\ \gamma_L &= \int dE f^\beta(E-\mu_L) \delta_L(E-H^{eff}) \\ \gamma_R &= \int dE f^\beta(E-\mu_R) \delta_R(E-H^{eff}) \end{aligned}$$

where μ_R and μ_L are now external parameters, typically expressed as

$$\mu_L = \mu + \frac{\Delta\mu}{2}$$

$$\mu_R = \mu - \frac{\Delta\mu}{2}$$

where $\mu = (\mu_L + \mu_R)/2$ is the equilibrium chemical potential, and $\Delta\mu$ is related to the ‘‘macroscopic’’ bias

$$\Delta\mu = -|e|V_{bias}$$

Thus, the non-equilibrium charge $\rho(\mathbf{x})$ in the scattering region used to build the effective Hamiltonian has to be consistent with the density matrix defined above, namely

$$\rho(\mathbf{x}) = \langle \mathbf{x} | \gamma | \mathbf{x} \rangle = \langle \mathbf{x} | \gamma_L | \mathbf{x} \rangle + \langle \mathbf{x} | \gamma_R | \mathbf{x} \rangle$$

This defines a self-consistent procedure which is of paramount importance to correctly describe *screening effects* within the scattering region. At self-consistency, H^{eff} (for a given $\Delta\mu$) is the effective Hamiltonian whose eigenvectors contain the scattering information needed to describe transport across the scattering region (for the given $\Delta\mu$).

6 Transmission probability and current

Having defined an effective Hamiltonian for a given non-equilibrium condition, we are in a position of computing the relevant scattering information. We are interested in the probability that an electron coming from the left electrode ends up in the right electrode, what can be called the *transmission probability*.

According to general scattering theory this probability is the expectation value of a *product-region flux operator* F which, in our case, reads as:

$$F_R = i [H, R] = i(HR - RH) = i(H_{CR} - H_{RC})$$

on account of the property $H_{LR} = H_{RL} = 0$. The probability that an electron in the state $|Ei, L\rangle$ “evolves” into the right electrode is then given by

$$P_i = 2\pi \langle Ei, L + | F_R | Ei, L + \rangle$$

where $|Ei, L + \rangle$ is the scattering eigenstate “evolved” from $|Ei, L\rangle$.

The total (or *cumulative*) transmission probability from left to right,

$$N_{R\leftarrow L}(E) = 2\pi \sum_i \langle Ei, L + | F_R | Ei, L + \rangle \equiv -4\pi \sum_i \text{Im} \langle Ei, L + | H_{CR} | Ei, L + \rangle$$

takes a simple form once

$$R |Ei, L + \rangle = g_R^+(E) H_{RC} G_{CC}^+(E) H_{CL} |Ei, L\rangle$$

$$C |Ei, L + \rangle = G_{CC}^+(E) H_{CL} |Ei, L\rangle$$

are introduced in the above expression and the sum is replaced by an appropriate trace operation. The trace is conveniently taken over the states in the scattering region, *e.g.* with the help of a basis $|\xi_k\rangle$ in C

$$N_{R\leftarrow L}(E) = -4\pi \sum_{i,k} \text{Im} [\langle Ei, L + | \xi_k \rangle \langle \xi_k | H_{CR} | Ei, L + \rangle]$$

$$\begin{aligned}
&= -4\pi \sum_{i,k} \text{Im} [\langle \xi_k | H_{CR} | Ei, L+ \rangle \langle Ei, L+ | \xi_k \rangle] \\
&= -4\pi \text{Im} [\text{Tr} (H_{CR} | Ei, L+ \rangle \langle Ei, L+ | C)] \\
&= -4\pi \text{Im} \left[\text{Tr} \left(H_{CR} g_R^+(E) H_{RC} G_{CC}^+(E) H_{CL} \sum_i | Ei, L+ \rangle \langle Ei, L+ | H_{LC} G_{CC}^-(E) \right) \right] \\
&= -4\pi \text{Im} [\text{Tr} (H_{CR} g_R^+(E) H_{RC} G_{CC}^+(E) H_{CL} \delta(E - H_{LL}) H_{LC} G_{CC}^-(E))]
\end{aligned}$$

Introducing

$$\Gamma_L(E) = 2\pi H_{CL} \delta(E - H_{LL}) H_{LC}$$

we arrive at

$$N_{R \leftarrow L}(E) = -2 \text{Im} [\text{Tr} (H_{CR} g_R^+(E) H_{RC} G_{CC}^+(E) \Gamma_L(E) G_{CC}^-(E))]]$$

The imaginary part is easily computed after noticing that

$$\begin{aligned}
\text{Tr} (H_{CR} g_R^+(E) H_{RC} G_{CC}^+(E) \Gamma_L(E) G_{CC}^-(E))^\dagger &= \text{Tr} (G_{CC}^+(E) \Gamma_L(E) G_{CC}^-(E) H_{CR} g_R^-(E) H_{RC}) \\
&= \text{Tr} (H_{CR} g_R^-(E) H_{RC} G_{CC}^+(E) \Gamma_L(E) G_{CC}^-(E))
\end{aligned}$$

thanks to the invariance under cyclic permutation of the trace operation, and reads as

$$N_{R \leftarrow L}(E) = \text{Tr} [H_{CR} (-2 \text{Im} g_R^-(E)) H_{RC} G_{CC}^+(E) \Gamma_L(E) G_{CC}^-(E)]$$

where $-2 \text{Im} g_R^-(E) = 2\pi \delta(E - H_{RR})$. Hence,

$$N_{R \leftarrow L}(E) = \text{Tr} [\Gamma_R(E) G_{CC}^+(E) \Gamma_L(E) G_{CC}^-(E)] \quad (16)$$

upon introducing $\Gamma_R(E) = 2\pi H_{CR} \delta(E - H_{RR}) H_{RC}$. Likewise,

$$N_{L \leftarrow R}(E) = \text{Tr} [\Gamma_L(E) G_{CC}^+(E) \Gamma_R(E) G_{CC}^-(E)] \quad (17)$$

These expressions take a suggestive form when the three operators on the right of the r.h.s. are recognized to be the density of left/right incoming states (see Eq.15),

$$N_{R \leftarrow L}(E) = 2\pi \text{Tr} [\Gamma_R(E) \delta_L(E - H^{eff})]$$

$$N_{L \leftarrow R}(E) = 2\pi \text{Tr} [\Gamma_L(E) \delta_R(E - H^{eff})]$$

In this form the cumulative transmission probability has the structure of a Fermi's golden rule expression, even though no perturbative approximations have been introduced.

Important simplifications arise when the Hamiltonian H is invariant under time-reversal (*i.e.* in absence of magnetic fields). In this case, the probability for the reverse process satisfies

$$N_{L \leftarrow R}(E) = N_{R \leftarrow L}(E)$$

Indeed, introducing the (anti-unitary) time-reversal operator⁸ T

$$\begin{aligned} N_{L\leftarrow R}(E) &= \text{Tr} \left[\Gamma_R(E) G_{CC}^-(E) \Gamma_L(E) G_{CC}^+(E) \right] = \text{Tr} \left[T^\dagger T \Gamma_R(E) G_{CC}^-(E) \Gamma_L(E) G_{CC}^+(E) \right] \\ &= \text{Tr} \left[T^\dagger \Gamma_R(E) G_{CC}^+(E) \Gamma_L(E) G_{CC}^-(E) T \right] = N_{R\leftarrow L}^*(E) = N_{R\leftarrow L}(E) \end{aligned}$$

Here we have used

$$T G_{CC}(\lambda) = T C (\lambda - H)^{-1} C = C (\lambda^* - H)^{-1} C T = G_{CC}(\lambda^*) T$$

and

$$\text{Tr}(T^\dagger A T) \equiv \sum_i \langle T \xi_i | A | T \xi_i \rangle^* = \sum_i \langle \xi_i | A | \xi_i \rangle^* = \text{Tr}(A)^*$$

as can be seen with the help of a basis of definite parity⁹, *e.g.* $|T \xi_i\rangle = |\xi_i\rangle$. Thus, under such circumstances, we can unambiguously refer to the *cumulative transmission probability*

$$N(E) = \text{Tr} \left(\Gamma_R(E) G_{CC}^+(E) \Gamma_L(E) G_{CC}^-(E) \right) \quad (18)$$

The *current* across the conductor can be computed with the help of the above results. The current $L \rightarrow R$ carried by the state $|Ei, L\rangle$ is given by

$$dI_{i,L} = -|e| n_L(E) P_i(E) v_i(E) \frac{dk}{2\pi}$$

where $n_L(E)$ is the occupation probability of the state ($\equiv f^\beta(E - \mu_L)$), $P_i(E)$ is the above transmission probability, $v_i(E) = \partial E / \partial k$ is electron velocity in this state and $dk/2\pi$ arises from the discretization of states in k -space,

$$\frac{dk}{2\pi} = \text{number of states for unit length} \times \text{number of states for unit } k$$

(the number of states for unit length times $n_L(E) P_i(E)$ defines the *linear density* of current-carrying electrons). Upon summing over i and noticing that $v_i(E) dk = dE$ irrespective of the dispersion relation (along the transport direction)

$$dI_L = -\frac{|e|}{h} n_L(E) N_{R\leftarrow L}(E) dE$$

⁸Such operator works similarly to a unitary operator, $T^\dagger T = T T^\dagger = 1$. The difference with a unitary operator is in its *anti-linear* property, $T(\lambda |\psi\rangle) = \lambda^* T |\psi\rangle$. This implies that $\langle \phi | T \psi \rangle = \langle T^\dagger \phi | \psi \rangle^*$ must hold if the ket and the bra positions have to be anti-linear.

⁹In general, for an arbitrary anti-unitary operator T , consider its eigenbasis, $T |\xi_k\rangle = t_k |\xi_k\rangle$ (where $|t_k| \equiv 1$) and write $t_k = e^{i2\phi_k}$, in such a way that $e^{-i\phi_k} T |\xi_k\rangle = T (e^{i\phi_k} |\xi_k\rangle) = (e^{i\phi_k} |\xi_k\rangle)$. For the time-reversal operator, idempotency $T^2 = 1$ fixes $\phi_k = 0, \pi/2$.

Hence, the total current from left to right reads as

$$I = -\frac{|e|}{h} \int_{-\infty}^{+\infty} dE \left[f^\beta(E - \mu_L) N_{R \leftarrow L}(E) - f^\beta(E - \mu_R) N_{L \leftarrow R}(E) \right]$$

on accounts of those electrons that starting from the right electrode ends up to the left one. Under time-reversal invariance the above expression simplifies to

$$I = -\frac{|e|}{h} \int_{-\infty}^{+\infty} dE N(E) (f^\beta(E - \mu_L) - f^\beta(E - \mu_R))$$

which provides the *characteristic I - V function* ($-|e|V \equiv (\mu_L - \mu_R)$).

In linear regime, *i.e.* for small bias $\delta\mu = \mu_L - \mu_R$, and at temperatures well below the Fermi temperatures of the electrodes, the Fermi factor is well peaked around the average chemical potential $\mu = (\mu_L + \mu_R)/2$,

$$f^\beta(E - \mu_L) - f^\beta(E - \mu_R) \approx -\frac{df^\beta}{d\mathcal{E}}(E - \mu)\delta\mu \approx \delta(E - \mu)\delta\mu$$

and the above expression further simplifies to

$$\delta I = \frac{|e|^2}{h} N(\mu)\delta V = G(\mu)\delta V$$

where $\delta\mu = -|e|\delta V$ has been used and the *(zero bias) conductance* (with the Fermi level positioned at μ)

$$G(\mu) = \frac{|e|^2}{h} N(\mu)$$

has been introduced. Thus, we can interpret $N(E)$ as the zero-bias conductance (in units of the *quantum of conductance* $|e|^2/h$) when the Fermi level is located at energy E , provided we disregard the effect that any *gate* potential may have on the effective Hamiltonian used to compute $N(E)$.

Alternatively, but always assuming that $N(E)$ does not depend on the bias, we can consider the *differential conductance* dI/dV

$$\begin{aligned} \frac{dI}{dV} &= -|e| \frac{dI}{d(\Delta\mu)} = \frac{|e|^2}{2} \int_{-\infty}^{+\infty} dE N(E) \frac{d}{d(\Delta\mu)} \left[f^\beta \left(E - \left(\bar{\mu} + \frac{\Delta\mu}{2} \right) \right) - f^\beta \left(E - \left(\bar{\mu} - \frac{\Delta\mu}{2} \right) \right) \right] \\ &= -\frac{|e|^2}{2} \int_{-\infty}^{+\infty} dE N(E) \frac{1}{2} \left[\frac{df^\beta}{d\mathcal{E}}(E - \mu_L) - \frac{df^\beta}{d\mathcal{E}}(E - \mu_R) \right] \end{aligned}$$

where $\frac{df^\beta}{dE}(E - \mu) \approx -\delta(E - \mu)$ and thus

$$\frac{dI}{dV} \cong \frac{|e|^2}{2} \frac{N(\mu_L) + N(\mu_R)}{2}$$

which obviously reduces to the previous result when the conductance is taken at zero bias ($\mu_L = \mu_R = \mu$). The above result also shows that, under the above hypothesis, $dI/dV > 0$, hence the *negative differential resistance* which is observed in some instances can only be due to the dependence of $N(E)$ on the applied bias.

Note

The careful reader may have noticed that naively applying the commutation relation entering in the flux definition one gets the absurd result that $P_i(E) = 0$. Indeed we know that for stationary states

$$-i \langle E_n | F_R | E_n \rangle = \langle E_n | H R - R H | E_n \rangle = E_n \langle E_n | R | E_n \rangle - E_n \langle E_n | R | E_n \rangle = 0$$

The point is that care is needed in computing matrix elements of operators between improper states.

Specifically, the probability is actually the result of the following limiting process

$$P_i(E) = \lim_{\epsilon \rightarrow 0^+} 2\pi \langle \psi_{E+i\epsilon}^{i,L} | F_R | \psi_{E+i\epsilon}^{i,L} \rangle = 2\pi i \lim_{\epsilon \rightarrow 0^+} \langle \psi_{E+i\epsilon}^{i,L} | H R - R H | \psi_{E+i\epsilon}^{i,L} \rangle$$

where $|\psi_\lambda^{i,L}\rangle$ solves the equation

$$(\lambda - H) |\psi_\lambda^{i,L}\rangle = (\lambda - H_{LL}) |Ei, L\rangle$$

i.e.

$$H |\psi_{E+i\epsilon}^{i,L}\rangle = (E + i\epsilon) |\psi_{E+i\epsilon}^{i,L}\rangle - i\epsilon |Ei, L\rangle$$

It follows (we write $|\psi_E^{i,L} + \rangle$ for $|\psi_{E+i\epsilon}^{i,L}\rangle$)

$$\begin{aligned} \langle \psi_E^{i,L} + | H R - R H | \psi_E^{i,L} + \rangle &= (E - i\epsilon) \langle \psi_E^{i,L} + | R | \psi_E^{i,L} + \rangle + i\epsilon \langle Ei, L | R | \psi_E^{i,L} + \rangle - \\ &- (E + i\epsilon) \langle \psi_E^{i,L} + | R | \psi_E^{i,L} + \rangle + i\epsilon \langle \psi_E^{i,L} + | R | Ei, L \rangle \end{aligned}$$

Here

$$i\epsilon \langle Ei, L | R | \psi_E^{i,L} + \rangle = i\epsilon \langle \psi_E^{i,L} + | R | Ei, L \rangle = 0$$

and thus we are left with

$$\langle \psi_E^{i,L} + | H R - R H | \psi_E^{i,L} + \rangle = -2i\epsilon \langle \psi_E^{i,L} + | R | \psi_E^{i,L} + \rangle$$

i.e.

$$P_i(E) = 4\pi \lim_{\epsilon \rightarrow 0^+} \epsilon \langle \psi_E^{i,L} + | R | \psi_E^{i,L} + \rangle$$

The limit is of course null only if $\langle \psi_E^{i,L} + |R|\psi_E^{i,L} \rangle$ remains finite for $\epsilon \rightarrow 0$, which is *not* the case here.

To see this we notice that the r.h.s is just the square modulus of the R projection of the improper state, and we explicitly have

$$\langle \psi_E^{i,L} + |R|\psi_E^{i,L} \rangle = \langle Ei, L | H_{LC} G_{CC}^-(E) H_{CR} g_R^-(E) g_R^+(E) H_{RC} G_{CC}^+(E) H_{CL} | Ei, L \rangle$$

where

$$g_R^-(E) g_R^+(E) = \frac{1}{E + i\epsilon - H_{RR}} \frac{1}{E - i\epsilon - H_{RR}} = \frac{1}{(E - H_{RR})^2 + \epsilon^2}$$

or equivalently

$$\lim_{\epsilon \rightarrow 0^+} \epsilon g_R^-(E) g_R^+(E) = \pi \delta(E - H_{RR})$$

This gives back the previous result

$$P_i(E) = 4\pi^2 \text{Tr} [G_{CC}^-(E) H_{CR} \delta(E - H_{RR}) H_{RC} G_{CC}^+(E) H_{CL} | Ei, L \rangle \langle Ei, L | H_{LC}]$$

here already written as a trace over states of the scattering region. Upon summing over i and introducing $\Gamma_R(E)$ and $\Gamma_L(E)$ as usual, one then obtains the above expression, Eq.16, for the cumulative transmission probability.