

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

Rocco Martinazzo

June 12, 2022

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.

Contents

1	The Green's operator	1
2	Green's operator for the (coupled) scattering region	5
3	Green's operators for the uncoupled electrodes	7
4	Scattering states	9
5	Self-consistency	11
6	Transmission probability and current	14
7	Note	18

1 The Green's operator

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 P_n when $E = E_n \in \sigma_d$ is a discrete eigenvalue (and the integral is just a sum), while it becomes

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

when E lies in the continuous spectrum σ_c . Here, $\{|E, i\rangle\}$ are improper eigenvectors at energy E and i is a degeneracy index. The operator $p(E)$ is a delta distribution on the spectral measure μ ,

$$p(E) \equiv \delta_{\mu}(E - H) = \begin{cases} \delta(E - H) & E \in \sigma_c \\ P_n & E = E_n \in \sigma_d \\ 0 & \text{otherwise} \end{cases}$$

that allows one to write any function of the operator H as a spectral integral with respect to the measure μ

$$f(H) = \int_{\sigma} f(E) \delta_{\mu}(E - H) d\mu_E$$

In the above expression, $\delta(E - H)$ is the **density-of-states operator** that is defined, in analogy to ordinary functions of the operators H , as¹

$$\delta(E - H) = \sum_n \delta(E - E_n) P_n + \chi_{\sigma_c}(E) \sum_i |E, i\rangle \langle E, i| \quad (1)$$

and is generally preferred over $\delta_{\mu}(E - H)$ since it allows one to re-write the spectral resolution as an *ordinary* integral over (any) set of energies containing the whole spectrum

$$f(H) = \int f(E) \delta(E - H) dE$$

For instance,

$$G(\lambda) = \int \frac{1}{\lambda - E} \delta(E - H) dE \equiv \int_{\sigma_c} \frac{1}{\lambda - E} \delta(E - H) dE + \sum_{\alpha} \frac{1}{\lambda - E_{\alpha}} P_{\alpha} \quad (2)$$

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)

¹In general, χ_A is the characteristic function of the set A .

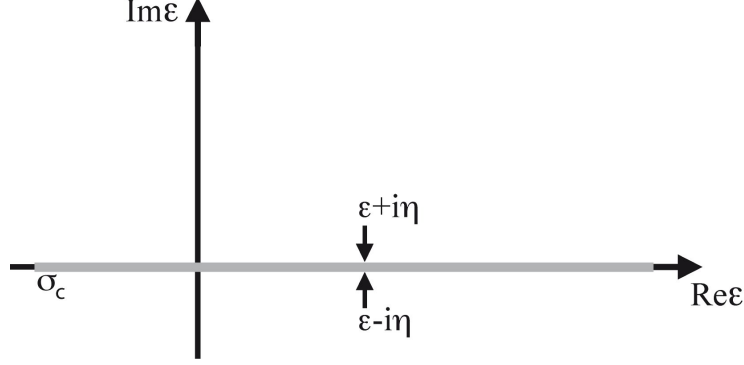


Figure 1: The limiting process on the complex energy plane described in the main text, here for $\lambda = \mathcal{E} \pm i\eta$.

$$\lim_{\epsilon \rightarrow 0^+} G(E \pm i\epsilon) = G^\pm(E) \quad (3)$$

for $E \in \sigma_c$. Indeed, from Eq. 2

$$G^+(E) - G^-(E) = \int_{\sigma_c} \left(\frac{1}{E + i\epsilon - E'} - \frac{1}{E - i\epsilon - E'} \right) \delta(E' - H) dE'$$

the term in brackets reads as

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

and, upon taking the limit $\epsilon \rightarrow 0^+$, gives

$$G^+(E) - G^-(E) = -2\pi i \delta(E - H) \quad (4)$$

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.

$$\boxed{\text{Im} G^+(E) = -\pi \delta(E - H)} \quad (5)$$

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:

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

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

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

Of course,

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

and thus³

$$\boxed{G^\pm(E) = G^P(E) \mp i\pi\delta(E - H)} \quad (6)$$

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

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

is well defined (convergent)⁴ and reads as

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

By the same token

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

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

$$\int_{\mathbb{R}} \Theta(\pm t) e^{i\lambda t} e^{-iHt} dt = \pm iG(\lambda) \quad \text{for } \lambda \in \mathbb{C}^\pm$$

³This equation actually holds for *any* $E \in \mathbb{R}$. If $E \in \mathbb{R}/\sigma$ the imaginary part vanishes and $G(E)$ is continuous across the real axis, $G^+(E) = G^-(E) = G^P(E)$. On the other hand, when the limit is taken (from any direction) to $E = E_n$ the function $G(\lambda)$ diverges as $(E - E_n)^{-1} P_n$ (see Eq.2), hence when approaching the discrete eigenvalue E_n the r.h.s. takes the form of a proper projector times a delta function, $\delta(E - E_n) P_n$, consistently with Eq.1.

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

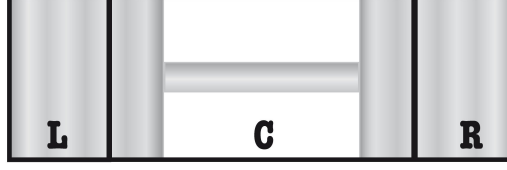


Figure 2: Setup for a two-terminal junction. L, R are the left and right electrodes, respectively, and C is the “conductor”.

where $\Theta(t) = 1$ for $t \geq 0$ and $\Theta(t) = 0$ otherwise. In particular,

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

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, thus making 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 expressions for the interesting quantities in terms of operators pertaining to the region C only. To this end, we first introduce the projection operators for the three regions, satisfying

$$R^2 = R = R^\dagger \quad C^2 = C = C^\dagger \quad L^2 = L = L^\dagger \\ RL = LC = RC = 0 \quad R + L + C = 1$$

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 $LHR = RHL = 0$ and obtain, upon taking the matrix elements between the space components,

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

We are interested in the set of equation of the middle-column G matrix

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

Solving for G_{LC} (G_{RC}) the first (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:

$$(\lambda - H_{\text{eff}}(\lambda))G_{CC}(\lambda) = C \quad (7)$$

where

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

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

$$H_{\text{eff}}(E) = H_{CC} + \Sigma_L^+(E) + \Sigma_R^+(E) \quad (8)$$

where

$$\boxed{\Sigma_L^+(E) = H_{CL}g_L^+(E)H_{LC} \quad \Sigma_R^+(E) = H_{CR}g_R^+(E)H_{RC}} \quad (9)$$

are the so-called electrode **self-energies**. 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

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

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

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

$$\boxed{H_{\text{eff}}(E) = H_{CC} + \Delta(E) - i\frac{\Gamma(E)}{2}} \quad (10)$$



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

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

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

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

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

The problem of determining $G_{CC}^+(E)$ thus boils down to the problem of computing the electrode self-energies and building up (and inverting) the effective Hamiltonian H_{eff} . 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 G_{LL} in place of g_L).

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

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

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

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 “short ranged” 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 $L_1 L_1$ 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 $g_{11}(\lambda)$

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

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 $(N-1)^{\text{th}}$ 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

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

where, for $n = 1, 2, \dots$,

$$\boxed{\begin{aligned} H_n^{\text{eff}}(\lambda) &= H_{nn} + \Sigma_n(\lambda) \\ \Sigma_n(\lambda) &= V_{n+1n}(\lambda - H_{n+1}^{\text{eff}}(\lambda))^{-1}V_{n+1n} \end{aligned}} \quad (12)$$

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

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

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

$$\mathbf{V}_{nm} = \langle \chi_n^{(1)} | V | \chi_m^{(2)} \rangle$$

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

$$\boxed{[\lambda - (\mathbf{H} + \mathbf{V}\mathbf{g}(\lambda)\mathbf{V}^\dagger)] \mathbf{g}(\lambda) = \mathbf{1}} \quad (13)$$

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 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

$$(\lambda - H) |\psi_\lambda\rangle = (\lambda - H_{\text{LL}}) |Ei, L\rangle \quad (14)$$

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,

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

i.e.,

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

The advantage of using the above limiting process in defining the eigenstate $|Ei, L+\rangle$ (compared to solving the eigenvalue equation) is that in that way one *explicitly* introduces the desired boundary condition, namely $|Ei, L+\rangle \rightarrow |Ei, L\rangle$ when the interaction $H - H_{\text{LL}}$ 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 the components of the scattering state in terms of the fundamental G_{CC}^+ Green’s function

$$\boxed{|\phi_R\rangle = g_R^+(E)H_{RC}G_{CC}^+(E)H_{CL} |Ei, L\rangle} \quad (15)$$

$$\boxed{|\phi_C\rangle = G_{CC}^+(E)H_{CL} |Ei, L\rangle} \quad (16)$$

$$\boxed{|\phi_L\rangle = |Ei, L\rangle + g_L^+(E)H_{LC}G_{CC}^+(E)H_{CL} |Ei, L\rangle} \quad (17)$$

where

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

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

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

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

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

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

where $\lim_{\epsilon \rightarrow 0^+} (E - H)G^+(E) = 1$ has 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 15-17, from $G_{CC}(E)$.

Computation of $G_{CC}(E)$ amounts to invert the operator $(E - H^{\text{eff}})$ 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 15-17 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 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

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

where $f^\beta(\epsilon)$ is the Fermi-Dirac occupation function

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

and $\delta(E - H^{\text{eff}})$ is the density-of-states operator of the scattering region. Then, according to Eq.5,

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

which is usually evaluated by exploiting the analytic properties of $G_{CC}(\lambda)$ (along with the meromorphic character of $f^\beta(\epsilon)$), namely by replacing the path along

⁶If $|i\rangle$ is eigenvector of H^{eff} with eigenvalue E_i then the vector $|\bar{i}\rangle$ must be eigenvector of $(H^{\text{eff}})^\dagger$ 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 $\langle\bar{i}| H^{\text{eff}} = \sum_j \langle\bar{i}| H^{\text{eff}} |j\rangle \langle\bar{j}| = \sum_j E_j \delta_{ij} \langle\bar{j}| = E_i \langle\bar{i}|$, and take the adjoint of this expression. The last equation shows that $\langle\bar{i}|$ is a left eigenvector of H^{eff} .

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 down the density-of-states operator in terms of the effective Hamiltonian H^{eff} by using

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

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

$$\delta(E - H^{\text{eff}}) = \frac{1}{2\pi} G_{CC}^+(E)\Gamma(E)G_{CC}^-(E) - \frac{1}{\pi} \lim_{\epsilon \rightarrow 0^+} \epsilon G_{CC}(E + i\epsilon)G_{CC}(E - i\epsilon)$$

Here the second term on the r.h.s. is really relevant only when $\Gamma(E)$ vanishes, as it happens, *e.g.*, for an isolated conductor (see also the Note at the end of this document). With this exception in mind we shall use

$$\boxed{\delta(E - H^{\text{eff}}) = \frac{1}{2\pi} G_{CC}^+(E)\Gamma(E)G_{CC}^-(E)} \quad (18)$$

in any other circumstances. Taking further into account that $\Gamma(E)$ has contributions from both the left and right electrodes, we end up with

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

where

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

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 (to the density operator) of those *states which evolved from the left electrode*

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

and similarly for the right-electrode contribution $\delta_R(E - H^{\text{eff}})$. Equivalently,

$$\boxed{\delta_L(E - H^{\text{eff}}) = \frac{1}{2\pi} G_{\text{CC}}^+(E) \Gamma_L(E) G_{\text{CC}}^-(E)} \quad (19)$$

and

$$\boxed{\delta_R(E - H^{\text{eff}}) = \frac{1}{2\pi} G_{\text{CC}}^+(E) \Gamma_R(E) G_{\text{CC}}^-(E)} \quad (20)$$

in close analogy with Eq. 18.

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

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

$$\gamma_L = \int dE f^\beta(E - \mu_L) \delta_L(E - H^{\text{eff}})$$

$$\gamma_R = \int dE f^\beta(E - \mu_R) \delta_R(E - H^{\text{eff}})$$

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

$$\mu_{L/R} = \mu \pm \frac{\Delta\mu}{2}$$

where $\mu = (\mu_L + \mu_R)/2$ is the equilibrium chemical potential, and $\Delta\mu$ relates to the “macroscopic” bias⁷

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

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

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

⁷Contrary to a common believe, a voltage probe always measures a difference in the chemical potential and only occasionally (*i.e.*, in the absence of a density gradient) this reduces to a difference in electrostatic potential.

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 is known as **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:

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

on account of the property $H_{\text{LR}} = H_{\text{RL}} = 0$. 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,

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

takes a simple form once

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

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

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

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

$$= -4\pi \text{Im} [\text{Tr} (H_{\text{CR}} g_{\text{R}}^+(E) H_{\text{RC}} G_{\text{CC}}^+(E) H_{\text{CL}} \delta(E - H_{\text{LL}}) H_{\text{LC}} G_{\text{CC}}^-(E))]$$

Introducing

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

(see Eq. 9) we arrive at

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

The imaginary part is easily computed upon noticing that

$$\begin{aligned} \text{Tr} (H_{\text{CR}} g_{\text{R}}^+(E) H_{\text{RC}} G_{\text{CC}}^+(E) \Gamma_{\text{L}}(E) G_{\text{CC}}^-(E))^\dagger &= \\ &= \text{Tr} (G_{\text{CC}}^+(E) \Gamma_{\text{L}}(E) G_{\text{CC}}^-(E) H_{\text{CR}} g_{\text{R}}^-(E) H_{\text{RC}}) \\ &= \text{Tr} (H_{\text{CR}} g_{\text{R}}^-(E) H_{\text{RC}} G_{\text{CC}}^+(E) \Gamma_{\text{L}}(E) G_{\text{CC}}^-(E)) \end{aligned}$$

holds thanks to the invariance under cyclic permutation of the trace operation. It reads as

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

where $-2\text{Im} g_{\text{R}}^-(E) = 2\pi \delta(E - H_{\text{RR}})$. It follows

$$\boxed{N_{R \leftarrow L}(E) = \text{Tr} [\Gamma_{\text{R}}(E) G_{\text{CC}}^+(E) \Gamma_{\text{L}}(E) G_{\text{CC}}^-(E)]} \quad (21)$$

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

$$\boxed{N_{L \leftarrow R}(E) = \text{Tr} [\Gamma_{\text{L}}(E) G_{\text{CC}}^+(E) \Gamma_{\text{R}}(E) G_{\text{CC}}^-(E)]} \quad (22)$$

These expressions take a suggestive form when the three rightmost operators on the r.h.s. are recognized to be the density of left/right incoming states (see Eq.20),

$$\begin{aligned} N_{R \leftarrow L}(E) &= 2\pi \text{Tr} [\Gamma_{\text{R}}(E) \delta_L(E - H^{\text{eff}})] \\ N_{L \leftarrow R}(E) &= 2\pi \text{Tr} [\Gamma_{\text{L}}(E) \delta_R(E - H^{\text{eff}})] \end{aligned}$$

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

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

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.

Here we have used

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

and

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

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**

$$N(E) = \text{Tr}(\Gamma_R(E)G_{CC}^+(E)\Gamma_L(E)G_{CC}^-(E)) \quad (23)$$

The **electric 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 $dk/2\pi$ is the number of electrons per unit length and per spin with k in the interval $(k, k + dk)$, so that

$$n_L(E) \times \frac{dk}{2\pi} \times v_i(E) = j_i(E)$$

is the (number) current density of electrons from band i (In general, $\mathbf{j}(\mathbf{k}) = d^D\mathbf{k}/(2\pi)^D \mathbf{v}(\mathbf{k})n(\epsilon_i(\mathbf{k}))$ is the corresponding current density in D dimensions. Notice that in 1D current density and *current* coincide). Upon summing over i and noticing that $v_i(E)dk = dE$ irrespective of the dispersion relation (along the transport direction)

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

⁹The argument applies for “spinless” electronic systems (or even-numbered many electron system), where $T^2 = 1$ holds in addition to unitarity. For anti-linear operators this condition does *not* constraint the eigenvalues of T , which in fact can be any number on the unit circle (contrarily to what happens for linear operators, for which idempotency implies that the possible eigenvalues are only ± 1). In fact, from $T|\xi\rangle = t|\xi\rangle$ it follows $T^2|\xi\rangle = |t|^2|\xi\rangle = |\xi\rangle$, i.e. $|t| = 1$ but this is already a consequence of unitarity (just notice that $\|T\xi\|^2 = |t|^2\|\xi\|^2$, where $\|T\xi\|^2 = \langle \xi | T^\dagger T \xi \rangle^* \equiv \|\xi\|^2$). As a matter of fact, an arbitrary phase-rotation of the vector $|\xi\rangle$ produces an eigenvector with a phase-rotated eigenvalue, $T(e^{i\phi}|\xi\rangle) = e^{-i\phi}t|\xi\rangle = te^{-i2\phi}(e^{i\phi}|\xi\rangle)$. Hence, upon setting $t = e^{i2\phi}$, we can always define an eigenvector with eigenvalue 1, $e^{-i\phi}T|\xi\rangle = T(e^{i\phi}|\xi\rangle) = (e^{i\phi}|\xi\rangle)$. For odd-numbered electron systems, on the other hand, $T^2 = -1$ prevents the existence of T -eigenvectors since $T^2|\xi\rangle = |t|^2|\xi\rangle = -|\xi\rangle$ (with $|t| = 1$) implies $|\xi\rangle = 0$. This is at the origin of the Kramers degeneracy. In this case, the trace mentioned in the text is conveniently taken on a Kramers-paired basis, and the result is the same.

Hence, the total current from left to right reads as

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

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** (here, $-|e|V \equiv (\mu_L - \mu_R)$).

In linear regime, that is 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 $\mu = (\mu_L + \mu_R)/2$,

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

and the above expression simplifies further 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

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

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

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

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

7 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 $|\psi_{E+i\epsilon}^{i,L}\rangle$)

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

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

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

that is,

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

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.21, for the cumulative transmission probability.