Transporte Quântico Mesoscópico

Quantum Matter Summer School - Materials & Concepts

Bruno Amorim

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Contents

1 Motivação

Seja

$$\begin{aligned} L &= \text{dimensão do dispositivo} \\ \ell_\phi &= \text{comprimento de coerência do electrão} \end{aligned}$$

(ℓ_ϕ é a distancia que o electrão se propaga em que a descrição de uma partícula é válida, isto é, a distância que se propaga sem interagir com outros electrões, fonões ou outras excitações do sistema)

Se

$$L \gg \ell_\phi,$$

podemos falar em condutividade como uma propriedade caracteristica do material e intensiva. Estamos no regime do transporte macroscópico.

Se

$$L \lesssim \ell_\phi,$$

propriedades de transporte dependem da geometria do dispositivo em particular. Apenas podemos falar em conductância. Estamos no regime mesoscópico.

2 Descrição de transporte como um problema de espalhamento

2.1 Sistema de dois terminais

Vamos considerar um sistema em que um dispositivo central está ligado a dois contactos eléctricos. Contactos estão ligados a uma bateria/fonte de voltagem. Descrever o sistema completo seria impraticável. Assumimos que aos contactos pode ser atribuido um potencial químico bem definido e constante no tempo (em analogia com mecânica de fluídos em vasos comunicantes).

2.2 Hamiltoniano

Uma aproximação comum é assumir que os contactos são infinitos e invariantes de translação. Então o sistema completo, é descrito pelo Hamiltoniano de tight-binding:

$$H = \begin{bmatrix} \ddots & \ddots & & & & & & & \\ \ddots & \boldsymbol{h}_L & \boldsymbol{v}_L & & & & & & \\ & \boldsymbol{v}_L^\dagger & \boldsymbol{h}_L & \boldsymbol{v}_{0,1} & & & & & \\ & & \boldsymbol{v}_{1,0} & \boldsymbol{h}_1 & \ddots & & & & \\ & & & \ddots & \ddots & \ddots & & & \\ & & & & \ddots & \boldsymbol{h}_N & \boldsymbol{v}_{N,N+1} & & \\ & & & & & \boldsymbol{v}_{N+1,N} & \boldsymbol{h}_R & \boldsymbol{v}_R & \\ & & & & & & \boldsymbol{v}_R^\dagger & \boldsymbol{h}_R & \ddots \\ & & & & & & & \ddots & \ddots \end{bmatrix}$$

$n = 1, ..., N$ é a região central

$n = 0, -1, ...$ é o contacto esquerdo

$$\begin{aligned} \boldsymbol{h}_0 = \boldsymbol{h}_{-1} = ... &= \boldsymbol{h}_L \\ \boldsymbol{v}_{-1,0} = \boldsymbol{v}_{-2,-1} = ... &= \boldsymbol{v}_L \\ \boldsymbol{v}_{0,-1} = \boldsymbol{v}_{-1,-2} = ... &= \boldsymbol{v}_L^\dagger \end{aligned}$$

$n = N+1, N+2, ...$ é o contacto direito

$$\begin{aligned}\boldsymbol{h}_{N+1} &= \boldsymbol{h}_{N+2} = ... = \boldsymbol{h}_R \\ \boldsymbol{v}_{N+1,N+2} &= \boldsymbol{v}_{N+2,N+3} = ... = \boldsymbol{v}_R \\ \boldsymbol{v}_{N+2,N+1} &= \boldsymbol{v}_{N+3,N+1} = ... = \boldsymbol{v}_R^\dagger\end{aligned}$$

2.3 Estados propagantes

Se os contactos fossem infinitos, teriamos estados propagantes (ou estados de Bloch). Estes satisfazem a equação de Schrödinger (no contacto esquerdo):

$$\boldsymbol{h}\Psi_n + \boldsymbol{v}\Psi_{n+1} + \boldsymbol{v}^\dagger\Psi_{n-1} = E\Psi_n.$$

Isto pode ser escrito em termos de uma matriz de transferência:

$$\begin{bmatrix} \mathbf{0} & \mathbf{1} \\ -\boldsymbol{v}^\dagger & (E-\boldsymbol{h}) \end{bmatrix} \begin{bmatrix} \Psi_{n-1} \\ \Psi_n \end{bmatrix} = \begin{bmatrix} \mathbf{1} & \mathbf{0} \\ \mathbf{0} & \boldsymbol{v} \end{bmatrix} \begin{bmatrix} \Psi_n \\ \Psi_{n+1} \end{bmatrix}.$$

Para estados propagantes, temos

$$\begin{bmatrix} \Psi_n \\ \Psi_{n+1} \end{bmatrix} = \lambda \begin{bmatrix} \Psi_{n-1} \\ \Psi_n \end{bmatrix},$$

de tal form que obtemos o problema de valores próprios generalizado ($Ax = \lambda Bx$):

$$\begin{bmatrix} \mathbf{0} & \mathbf{1} \\ -\boldsymbol{v}_L^\dagger & (E-\boldsymbol{h}_L) \end{bmatrix} \begin{bmatrix} \Psi_{n-1} \\ \Psi_n \end{bmatrix} = \lambda \begin{bmatrix} \mathbf{1} & \mathbf{0} \\ \mathbf{0} & \boldsymbol{v}_L \end{bmatrix} \begin{bmatrix} \Psi_{n-1} \\ \Psi_n \end{bmatrix}.$$

Para estados propagantes: $|\lambda| = 1 \Rightarrow \lambda_\pm = e^{\pm ika}$.

2.3.1 Operador de currente para estados propagantes

O operador corrente é definido como

$$\frac{d\rho_n}{dt} = I_{n-1\to n} - I_{n\to n+1}$$

É facil de ver que

$$I_{n\to n+1} = \frac{i}{\hbar}\begin{bmatrix} \mathbf{0} & \boldsymbol{v}_{n,n+1} \\ -\boldsymbol{v}_{n+1,n} & \mathbf{0} \end{bmatrix}.$$

Para estados propagantes, obtemos

$$\begin{aligned}\langle \mathbf{\Phi}| I_{n\to n+1} |\mathbf{\Psi}\rangle &= \frac{i}{\hbar}\left(\Phi_n^\dagger \boldsymbol{v}_{n,n+1}\Psi_{n+1} - \Phi_{n+1}^\dagger \boldsymbol{v}_{n+1,n}\Psi_n\right) \\ &= \frac{i}{\hbar}\Phi_n^\dagger\left(\lambda_\Psi \boldsymbol{v}_{n,n+1} - \lambda_\Phi^* \boldsymbol{v}_{n+1,n}\right)\Psi_n\end{aligned}$$

2.3.2 Ortogonalidade de estados propagantes

Consideremos dois estados propagantes:

$$\begin{aligned}\left(\lambda_\Psi \boldsymbol{v}_L + \lambda_\Psi^{-1}\boldsymbol{v}_L^\dagger\right)\Psi_n &= (E-\boldsymbol{h}_L)\Psi_n \\ \left(\lambda_\Phi \boldsymbol{v}_L + \lambda_\Phi^{-1}\boldsymbol{v}_L^\dagger\right)\Phi_n &= (E-\boldsymbol{h}_L)\Phi_n\end{aligned}$$

Tomar hermítico conjugado da segunda equação e actuar com Ψ_n:

$$\Phi_n^\dagger\left(\lambda_\Phi^* \boldsymbol{v}_L^\dagger + (\lambda_\Phi^*)^{-1}\boldsymbol{v}_L\right)\Psi_n = \Phi_n^\dagger (E-\boldsymbol{h}_L)\Psi_n = \Phi_n^\dagger\left(\lambda_\Psi \boldsymbol{v}_L + \lambda_\Psi^{-1}\boldsymbol{v}_L^\dagger\right)\Psi_n$$

Podemos escrever isto como

$$\left[\lambda_\Phi^* - \lambda_\Psi^{-1}\right]\Phi_n^\dagger \boldsymbol{v}_L^\dagger \Psi_n = \left[\lambda_\Psi - (\lambda_\Phi^*)^{-1}\right]\Phi_n^\dagger \boldsymbol{v}_L \Psi_n$$

Multiplicando por $\lambda_\Psi \lambda_\Phi^*$ obtemos

$$[\lambda_\Psi \lambda_\Phi^* - 1]\, \lambda_\Phi^* \Phi_n^\dagger \boldsymbol{v}_L^\dagger \Psi_n = [\lambda_\Psi \lambda_\Phi^* - 1]\, \lambda_\Psi \Phi_n^\dagger \boldsymbol{v}_L \Psi_n$$

o que pode ser escrito como

$$[\lambda_\Psi \lambda_\Phi^* - 1]\, \Phi_n^\dagger \left(\lambda_\Psi \boldsymbol{v}_L \Psi_n - \lambda_\Phi^* \boldsymbol{v}_L^\dagger\right) \Psi_n = 0.$$

Se

$$\lambda_\Psi \lambda_\Phi^* \neq 1,$$

temos que

$$\langle \boldsymbol{\Phi}|\, I_{n\to n+1}\, |\boldsymbol{\Psi}\rangle = \frac{i}{\hbar} \Phi_n^\dagger \left(\lambda_\Psi \boldsymbol{v}_L - \lambda_\Phi^* \boldsymbol{v}_L^\dagger\right) \Psi_n = 0.$$

Para o caso em que

$$\lambda_\Psi \lambda_\Phi^* = 1,$$

podemos escolher

$$\langle \boldsymbol{\Phi}|\, I_{n\to n+1}\, |\boldsymbol{\Psi}\rangle = \frac{i}{\hbar} \Phi_n^\dagger \left(\lambda_\Psi \boldsymbol{v}_L - \lambda_\Phi^* \boldsymbol{v}_L^\dagger\right) \Psi_n = v_\Psi \delta_{\Psi,\Phi}.$$

2.4 Estados de espalhamento

Estado propagante para a direita:

$$|\Psi_{+,\alpha}\rangle = \begin{cases} \left|\Psi^+_{L,+,\alpha}\right\rangle + \sum_\beta r^{R\leftarrow L}_{\beta\alpha} \left|\Psi_{L,-,\beta}\right\rangle & ,\text{contacto esquerdo} \\ ? & ,\ \text{região central} \\ \sum_\gamma t^{R\leftarrow L}_{\gamma\alpha} \left|\Psi_{R,+,\gamma}\right\rangle & ,\ \text{contacto direito} \end{cases}$$

Estado propagante para a esquerda

$$|\Psi_{-,\gamma}\rangle = \begin{cases} \sum_\alpha t^{L\leftarrow R}_{\alpha\gamma} \left|\Psi^-_{L,\alpha}\right\rangle & ,\text{contacto esquerdo} \\ ? & ,\ \text{região central} \\ \left|\Psi_{R,-,\gamma}\right\rangle + \sum_\delta r^{L\leftarrow R}_{\delta\gamma} \left|\Psi^+_{R,+,\delta}\right\rangle & ,\ \text{contacto direito} \end{cases}$$

Notar que conservação do fluxo de probabilidade, implica que

$$\begin{aligned} v_{\alpha,L} &= \sum_\beta v_{\beta,L} \left|r^{R\leftarrow L}_{\beta\alpha}\right|^2 + \sum_\gamma v_{\gamma,R} \left|t^{R\leftarrow L}_{\gamma\alpha}\right|^2 \\ v_{\gamma,R} &= \sum_\delta v_{\delta,L} \left|r^{L\leftarrow R}_{\delta\gamma}\right|^2 + \sum_\alpha v_{\alpha,R} \left|t^{L\leftarrow R}_{\alpha\gamma}\right|^2 \end{aligned}$$

Mais genericamente:

$$\begin{bmatrix} \sqrt{\frac{v_{\alpha,L}}{v_{\beta,L}}} r^{R\leftarrow L}_{\alpha\beta} & \sqrt{\frac{v_{\alpha,L}}{v_{\delta,R}}} t^{L\leftarrow R}_{\alpha\delta} \\ \sqrt{\frac{v_{\gamma,R}}{v_{\beta,L}}} t^{R\leftarrow L}_{\gamma\beta} & \sqrt{\frac{v_{\gamma,R}}{v_{\delta,R}}} r^{L\leftarrow R}_{\gamma\delta} \end{bmatrix} \begin{bmatrix} \Psi^+_{L,\beta}(E) \\ \Psi^-_{R,\delta}(E) \end{bmatrix} = \begin{bmatrix} \Psi^-_{L,\alpha}(E) \\ \Psi^+_{R,\gamma}(E) \end{bmatrix}$$

é unitária.

2.5 Fórmula de Landauer-Buttiker

Para obtermos a fórmula de Landauer-Buttiker, podemos fazer a seguinte argumentação:

1) a ocupação dos estados propagantes para a direita (esquerda) é controlada pelo potencial químico do contacto esquerdo (direito).

Vamos medir a currente no contacto direito.

A corrente devido a um estado $|\Psi_\alpha^+(E)\rangle$ é

$$\begin{aligned}
I_{L\to R}(E,\alpha) &= \left\langle \Psi_\alpha^+(E)\right| I_{N+1\to N+2}\left|\Psi_\alpha^+(E)\right\rangle \\
&= \sum_{\gamma,\delta}\left(t_{\delta\alpha}^{R\leftarrow L}\right)^* t_{\gamma\alpha}^{R\leftarrow L}\left\langle \Psi_{R,\delta}^+(E)\right| I_{N+1\to N+2}\left|\Psi_{R,\gamma}^+(E)\right\rangle \\
&= \sum_{\gamma,\delta}\left(t_{\delta\alpha}^{R\leftarrow L}\right)^* t_{\gamma\alpha}^{R\leftarrow L} v_{\gamma,R}\delta_{\gamma,\delta} \\
&= \sum_{\gamma} v_{\gamma,R}\left|t_{\gamma\alpha}^{R\leftarrow L}\right|^2 .
\end{aligned}$$

Somando sobre todos os estados propagantes para a direita, obtemos

$$I_{L\to R}^+ = \sum_\alpha \int \frac{dk(E)}{2\pi} f_L(E) I_{L\to R}(E,\alpha).$$

Transformando o integral sobre k num integral sobre energia

$$dk(E) = dE\frac{dk}{dE} = dE\frac{1}{\hbar v_{\alpha,L}}$$

obtemos então

$$I_{L\to R}^+ = \frac{1}{\hbar}\sum_{\alpha,\gamma}\int \frac{dE}{2\pi} f_L(E)\frac{v_{\gamma,R}}{v_{\alpha,L}}\left|t_{\gamma\alpha}^{R\leftarrow L}\right|^2 .$$

A corrente devido a um estado $\left|\Psi_\gamma^-(E)\right\rangle$ é

$$\begin{aligned}
I_{L\to R}(E,\gamma) &= \left\langle \Psi_\gamma^-(E)\right| I_{N+1\to N+2}\left|\Psi_\gamma^-(E)\right\rangle \\
&= \left\langle \Psi_\gamma^-(E)\right| I_{N+1\to N+2}\left|\Psi_{R,\gamma}^-(E)\right\rangle - e\sum_{\delta,\delta'}\left(r_{\delta'\gamma}^{L\leftarrow R}\right)^* r_{\delta\gamma}^{L\leftarrow R}\left\langle \Psi_{R,\delta'}^+(E)\right| I_{N+1\to N+2}\left|\Psi_{R,\delta}^+(E)\right\rangle \\
&= \left(-v_{\gamma,R} + \sum_\delta v_{\delta,R}\left|r_{\delta\gamma}^{L\leftarrow R}\right|^2\right) \\
&= e\sum_\alpha v_{\alpha,L}\left|t_{\alpha\gamma}^{L\leftarrow R}\right|^2
\end{aligned}$$

Obtemos então

$$I_{L\to R}^- = \frac{1}{\hbar}\sum_{\alpha,\gamma}\int \frac{dE}{2\pi} f_R(E)\frac{v_{\alpha,L}}{v_{\gamma,R}}\left|t_{\alpha\gamma}^{L\leftarrow R}\right|^2 .$$

Temos então

$$\begin{aligned}
I_{L\to R} &= I_{L\to R}^+ - I_{L\to R}^- \\
&= \frac{1}{\hbar}\sum_{\alpha,\gamma}\int \frac{dE}{2\pi}\left(f_L(E)\frac{v_{\gamma,R}}{v_{\alpha,L}}\left|t_{\gamma\alpha}^{R\leftarrow L}\right|^2 - f_R(E)\frac{v_{\alpha,L}}{v_{\gamma,R}}\left|t_{\alpha\gamma}^{L\leftarrow R}\right|^2\right).
\end{aligned}$$

Em equilíbrio termodinâmico a corrente tem de ser zero, logo obtemos a seguinte relação

$$\frac{v_{\gamma,R}}{v_{\alpha,L}}\left|t_{\gamma\alpha}^{R\leftarrow L}\right|^2 = \frac{v_{\alpha,L}}{v_{\gamma,R}}\left|t_{\alpha\gamma}^{L\leftarrow R}\right|^2 .$$

O que nos permite escrever

$$I_{L\to R}^e = -\frac{e}{\hbar}\int \frac{dE}{2\pi}\left(f_L(E) - f_R(E)\right)\sum_{\alpha,\gamma}\frac{v_{\gamma,R}}{v_{\alpha,L}}\left|t_{\gamma\alpha}^{R\leftarrow L}\right|^2 .$$

2.6 Como calcular coefficientes de transmissão

Estados propagantes são solução da equação de Schrödinger:

$$\begin{bmatrix}
\ddots & \ddots & & & & & & & \\
\ddots & \boldsymbol{h}_L - E & \boldsymbol{v}_L & & & & & & \\
& \boldsymbol{v}_L^{\dagger} & \boldsymbol{h}_L - E & \boldsymbol{v}_{0,1} & & & & & \\
& & \boldsymbol{v}_{1,0} & \boldsymbol{h}_1 - E & \ddots & & & & \\
& & & \ddots & \ddots & \ddots & & & \\
& & & & \ddots & \boldsymbol{h}_N - E & \boldsymbol{v}_{N,N+1} & & \\
& & & & & \boldsymbol{v}_{N+1,N} & \boldsymbol{h}_R - E & \boldsymbol{v}_R & \\
& & & & & & \boldsymbol{v}_R^{\dagger} & \boldsymbol{h}_R - E & \ddots \\
& & & & & & & \ddots & \ddots
\end{bmatrix}
\begin{bmatrix}
\vdots \\ \Psi_{-1} \\ \Psi_0 \\ \Psi_1 \\ \vdots \\ \Psi_N \\ \Psi_{N+1} \\ \Psi_{N+2} \\ \vdots
\end{bmatrix} = 0$$

Será que conseguimos reduzir a matriz infinita a uma matriz infinita?

Temos:

$$\begin{aligned}
-\boldsymbol{v}_L^{\dagger}\Psi_{-1} + (E - \boldsymbol{h}_L)\,\Psi_0 - \boldsymbol{v}_{0,1}\Psi_1 &= 0 \\
-\boldsymbol{v}_{1,0}\Psi_0 + (E - \boldsymbol{h}_1)\,\Psi_1 - \boldsymbol{v}_{1,2}\Psi_2 &= 0 \\
&\vdots \\
-\boldsymbol{v}_{N,N-1}\Psi_{N-1} + (E - \boldsymbol{h}_N)\,\Psi_N - \boldsymbol{v}_R\Psi_{N+1} &= 0 \\
-\boldsymbol{v}_{N+1,N}\Psi_N + (E - \boldsymbol{h}_R)\,\Psi_{N+1} - \boldsymbol{v}_R\Psi_{N+2} &= 0
\end{aligned}$$

Vamos definir

$$\begin{aligned}
\Psi_{L,\alpha,+,n+m} &= \boldsymbol{F}_{L,+}^{m}\Psi_{L,\alpha,+,n} \\
\Psi_{L,\alpha,-,n+m} &= \boldsymbol{F}_{L,-}^{m}\Psi_{L,\alpha,-,n}
\end{aligned}$$

Donde obtemos:

$$\begin{aligned}
\boldsymbol{F}_{L,+} &= \boldsymbol{\Psi}_{L,+}\cdot\boldsymbol{\Lambda}_{L,+}\cdot\boldsymbol{\Psi}_{L,+}^{-1} \\
\boldsymbol{F}_{L,-} &= \boldsymbol{\Psi}_{L,-}\cdot\boldsymbol{\Lambda}_{L,-}\cdot\boldsymbol{\Psi}_{L,-}^{-1}
\end{aligned}$$

Isto permite escrever

$$\begin{aligned}
\Psi_0 &= \Psi_0^{+} + \Psi_0^{-} \\
\Psi_{-1} &= \Psi_{-1}^{+} + \Psi_{-1}^{-} \\
&= \boldsymbol{F}_{L,+}^{-1}\Psi_0^{+} + \boldsymbol{F}_{L,-}^{-1}\Psi_0^{-}
\end{aligned}$$

Fixamos Ψ_0^{+}, de tal foma que $\Psi_0^{-} = \Psi_0 - \Psi_0^{+}$.

Logo podemos escrever:

$$-\boldsymbol{v}_L^{\dagger}\Psi_{-1} + (E - \boldsymbol{h}_L)\,\Psi_0 - \boldsymbol{v}_{0,1}\Psi_1 = 0$$

Escrevemos

$$\begin{aligned}
\Psi_{-1} &= \Psi_{-1}^{+} + \Psi_{-1}^{-} \\
&= \boldsymbol{F}_{L,+}^{-1}\Psi_0^{+} + \boldsymbol{F}_{L,-}^{-1}\Psi_0^{-} \\
&= \boldsymbol{F}_{L,+}^{-1}\Psi_0^{+} + \boldsymbol{F}_{L,-}^{-1}\left(\Psi_0 - \Psi_0^{+}\right)
\end{aligned}$$

Desta forma a equação:

$$-\boldsymbol{v}_L^{\dagger}\Psi_{-1} + (E - \boldsymbol{h}_L)\,\Psi_0 - \boldsymbol{v}_{0,1}\Psi_1 = 0$$

Pode ser escrita como

$$-\boldsymbol{v}_L^\dagger \left[\boldsymbol{F}_{L,+}^{-1}\Psi_0^+ + \boldsymbol{F}_{L,-}^{-1}\left(\Psi_0 - \Psi_0^+\right)\right] + \left(E - \boldsymbol{h}_L\right)\Psi_0 - \boldsymbol{v}_{0,1}\Psi_1 = 0$$

$$\left(E - \boldsymbol{h}_L - \boldsymbol{v}_L^\dagger \boldsymbol{F}_{L,-}^{-1}\right)\Psi_0 - \boldsymbol{v}_{0,1}\Psi_1 = \boldsymbol{v}_L^\dagger \left[\boldsymbol{F}_{L,+}^{-1} - \boldsymbol{F}_{L,-}^{-1}\right]\Psi_0^+$$

Logo obtemos

$$\left(E - \boldsymbol{h}_L - \boldsymbol{v}_L^\dagger \boldsymbol{F}_{L,-}^{-1}\right)\Psi_0 - \boldsymbol{v}_{0,1}\Psi_1 = +\boldsymbol{v}_L^\dagger \left[\boldsymbol{F}_{L,-}^{-1} - \boldsymbol{F}_{L,+}^{-1}\right]\Psi_0^+$$

Vamos definir

$$\boldsymbol{\Sigma}_L^R = \boldsymbol{v}_L^\dagger \boldsymbol{F}_{L,-}^{-1}$$
$$\boldsymbol{\Sigma}_L^A = \boldsymbol{v}_L^\dagger \boldsymbol{F}_{L,+}^{-1}$$

De igual forma

$$\Psi_{N+2} = \Psi_{N+2}^+ = \boldsymbol{F}_{R,+}\Psi_{N+1}^+$$

De tal forma que

$$-\boldsymbol{v}_{N+1,N}\Psi_N + \left(E - \boldsymbol{h}_R\right)\Psi_{N+1} - \boldsymbol{v}_R \boldsymbol{F}_{R,+}\Psi_{N+1} = 0$$
$$-\boldsymbol{v}_{N+1,N}\Psi_N + \left(E - \boldsymbol{h}_R - \boldsymbol{v}_R \boldsymbol{F}_{R,+}\right)\Psi_{N+1} = 0$$

Definir

$$\boldsymbol{\Sigma}_R^R = \boldsymbol{v}_R \boldsymbol{F}_{R,+}$$

De tal forma que obtemos

$$\begin{bmatrix} E - \boldsymbol{h} - \boldsymbol{\Sigma}_L^R & -\boldsymbol{v}_{0,1} & & & \\ -\boldsymbol{v}_{1,0} & E - \boldsymbol{h}_1 & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & E - \boldsymbol{h}_N & -\boldsymbol{v}_{N,N+1} \\ & & & -\boldsymbol{v}_{N+1,N} & E - \boldsymbol{h}_R - \boldsymbol{\Sigma}_L^R \end{bmatrix} \begin{bmatrix} \Psi_0 \\ \Psi_1 \\ \vdots \\ \Psi_N \\ \Psi_{N+1} \end{bmatrix} = \begin{bmatrix} i\boldsymbol{\Gamma_L}\Psi_0^+ \\ 0 \\ \vdots \\ 0 \\ 0 \end{bmatrix}$$

Designar:

$$\left[\boldsymbol{G}^R\right]^{-1} = \begin{bmatrix} E - \boldsymbol{h} - \boldsymbol{\Sigma}_L^R & -\boldsymbol{v}_{0,1} & & & \\ -\boldsymbol{v}_{1,0} & E - \boldsymbol{h}_1 & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & E - \boldsymbol{h}_N & -\boldsymbol{v}_{N,N+1} \\ & & & -\boldsymbol{v}_{N+1,N} & E - \boldsymbol{h}_R - \boldsymbol{\Sigma}_L^R \end{bmatrix}.$$

De tal forma que

$$\Psi_{N+1} = i\boldsymbol{G}_{N+1,0}^R \boldsymbol{\Gamma}_L \Psi_0^+.$$

Projectar no estados transmitions:

$$t_{\gamma\alpha}^{R\leftarrow L} = i\Psi_{R,+,\gamma}^{-1}\boldsymbol{G}_{N+1,0}^R \boldsymbol{\Gamma}_L \Psi_{L,\alpha}^+$$

Onde $\Psi_{R,+,\gamma}^{-1}$ são as linhas da matriz, definida tal que

$$\boldsymbol{\Psi}_{R,+}^{-1} \cdot \boldsymbol{\Psi}_{R,+} = \mathbf{1}.$$

2.7 Matriz Γ como operador de currente na base de estados propagantes.

Primeiro vamos ver que

$$\left[\boldsymbol{v}_L^\dagger \boldsymbol{F}_{L,+}^{-1}\right]^\dagger = \boldsymbol{v}_L^\dagger \boldsymbol{F}_{L,-}^{-1}$$

Vamos então estudar

$$\begin{aligned}\left[\boldsymbol{v}_L^\dagger \boldsymbol{F}_{L,+}^{-1}\right]^\dagger - \boldsymbol{v}_L^\dagger \boldsymbol{F}_{L,-}^{-1} &= \left[\boldsymbol{v}^\dagger \boldsymbol{\Psi}_+ \cdot \boldsymbol{\Lambda}_+^{-1} \cdot \boldsymbol{\Psi}_+^{-1}\right]^\dagger - \boldsymbol{v}^\dagger \boldsymbol{\Psi}_- \cdot \boldsymbol{\Lambda}_-^{-1} \cdot \boldsymbol{\Psi}_-^{-1} \\ &= \left[\boldsymbol{\Psi}_+^\dagger\right]^{-1} \cdot \left[\boldsymbol{\Lambda}_+^\dagger\right]^{-1} \cdot \boldsymbol{\Psi}_+^\dagger \cdot \boldsymbol{v} - \boldsymbol{v}^\dagger \boldsymbol{\Psi}_- \cdot \boldsymbol{\Lambda}_-^{-1} \cdot \boldsymbol{\Psi}_-^{-1}\end{aligned}$$

Actuar com $\boldsymbol{\Psi}_+^\dagger$ e $\boldsymbol{\Psi}_-$:

$$\left[\boldsymbol{\Lambda}_+^\dagger\right]^{-1} \cdot \boldsymbol{\Psi}_+^\dagger \cdot \boldsymbol{v} \cdot \boldsymbol{\Psi}_- - \boldsymbol{\Psi}_+^\dagger \cdot \boldsymbol{v}^\dagger \cdot \boldsymbol{\Psi}_- \cdot \boldsymbol{\Lambda}_-^{-1}$$

entrada α, β da matriz

$$\Psi_{\alpha,+}^\dagger \left[\left(\lambda_{\alpha,+}^*\right)^{-1} \boldsymbol{v} - \boldsymbol{v}^\dagger \lambda_{\beta,-}^{-1}\right] \Psi_{\beta,-}$$

Multiplicar por $\lambda_{\alpha,+}^* \lambda_{\beta,-}$:

$$\Psi_{\alpha,+}^\dagger \left[\lambda_{\beta,-} \boldsymbol{v} - \lambda_{\alpha,+}^* \boldsymbol{v}^\dagger\right] \Psi_{\beta,-} = -i \left\langle \Psi_{\alpha,+} \right| I_{-1\to 0} \left| \Psi_{\beta,-} \right\rangle = 0$$

$$\left\langle \boldsymbol{\Phi} \right| I_{n+1\to n+2} \left| \boldsymbol{\Psi} \right\rangle = i \Phi_n^\dagger \left(\lambda_\Psi \boldsymbol{v}_L \Psi_n - \lambda_\Phi^* \boldsymbol{v}_L^\dagger\right) \Psi_n = v_\Psi \delta_{\Psi,\Phi}$$

Logo podemos escrever

$$\left(\boldsymbol{\Sigma}_L^R\right)^\dagger = \boldsymbol{\Sigma}_L^A$$

e

$$\boldsymbol{\Gamma}_L = i \left[\left[\boldsymbol{\Psi}_{L,+}^\dagger\right]^{-1} \cdot \left[\boldsymbol{\Lambda}_{L,+}^\dagger\right]^{-1} \cdot \boldsymbol{\Psi}_{L,+}^\dagger \cdot \boldsymbol{v}_L - \boldsymbol{v}_L^\dagger \boldsymbol{\Psi}_{L,+} \cdot \boldsymbol{\Lambda}_{L,+}^{-1} \cdot \boldsymbol{\Psi}_{L,+}^{-1}\right]$$

Actuar com

$$\begin{aligned}\Psi_{L,\alpha,+}^\dagger \boldsymbol{\Gamma}_L \Psi_{L,\beta,+} &= i \Psi_{L,\alpha,+}^\dagger \left[\left(\lambda_{L,+,\alpha}^*\right)^{-1} \boldsymbol{v}_L - \boldsymbol{v}_L^\dagger \lambda_{L,+,\beta}^{-1}\right] \Psi_{L,\beta,+} \\ &= \frac{1}{\lambda_{L,+,\alpha}^* \lambda_{L,+,\beta}} i \Psi_{L,\alpha,+}^\dagger \left[\lambda_{L,+,\beta} \boldsymbol{v}_L - \boldsymbol{v}_L^\dagger \lambda_{L,+,\alpha}^*\right] \Psi_{L,\beta,+} \\ &= \frac{1}{\lambda_{L,+,\alpha}^* \lambda_{L,+,\beta}} \hbar v_\alpha \delta_{\alpha,\beta}\end{aligned}$$

Para estados propagantes $\left|\lambda_{L,+,\alpha}\right|^2 = 1$ e logo

$$\begin{aligned}\boldsymbol{\Gamma} &= \hbar \left[\boldsymbol{\Psi}^\dagger\right]^{-1} \cdot \boldsymbol{V} \cdot \boldsymbol{\Psi}^{-1} \\ \boldsymbol{\Gamma}^{-1} &= \frac{1}{\hbar} \boldsymbol{\Psi} \cdot \boldsymbol{V}^{-1} \cdot \boldsymbol{\Psi}^\dagger\end{aligned}$$

e

$$\boldsymbol{\Psi}^{-1} = \frac{1}{\hbar} \boldsymbol{V}^{-1} \boldsymbol{\Psi}^\dagger \boldsymbol{\Gamma}.$$

Os coefficientes de transmissão podem então ser escritos como:

$$\begin{aligned}t_{\gamma\alpha}^{R\leftarrow L} &= i \left[\Psi_{R,\gamma}^\dagger\right]^{-1} \boldsymbol{G}_{N+1,0}^R \boldsymbol{\Gamma}_L \Psi_{L,\alpha}^+ \\ &= \frac{i}{\hbar v_{R,\gamma}} \Psi_{R,\gamma,+}^\dagger \boldsymbol{\Gamma}_R \boldsymbol{G}_{N+1,0}^R \boldsymbol{\Gamma}_L \Psi_{L,\alpha,+}\end{aligned}$$

Os coeficientes de transmissão reescalados, tomam a forma (relação de Fisher-Lee)

$$\tilde{t}_{\gamma\alpha}^{R\leftarrow L} = \sqrt{\frac{v_{\gamma,R}}{v_{\alpha,L}}} t_{\gamma\alpha}^{R\leftarrow L} = \frac{i}{\hbar\sqrt{v_{R,\gamma} v_{\alpha,L}}} \Psi_{R,\gamma,+}^\dagger \boldsymbol{\Gamma}_R \boldsymbol{G}_{N+1,0}^R \boldsymbol{\Gamma}_L \Psi_{L,\alpha,+}.$$

In matrix form

$$\tilde{\boldsymbol{t}}^{R\leftarrow L} = \frac{i}{\hbar} \boldsymbol{V}_R^{-1/2} \boldsymbol{\Psi}_{R,+}^\dagger \boldsymbol{\Gamma}_R \boldsymbol{G}_{N+1,0}^R \boldsymbol{\Gamma}_L \boldsymbol{\Psi}_{L,+} \boldsymbol{V}_L^{-1/2}$$

Transmissão:

$$\begin{aligned}
\mathcal{T}(E) &= \sum_{\gamma\alpha} \frac{v_{\gamma,R}}{v_{\alpha,L}} \left| t_{\gamma\alpha}^{R\leftarrow L} \right|^2 \\
&= \sum_{\gamma\alpha} \frac{1}{\hbar v_{R,\gamma} \hbar v_{\alpha,L}} \Psi_{R,\gamma,+}^{\dagger} \boldsymbol{\Gamma}_R \boldsymbol{G}_{N+1,0}^{R} \boldsymbol{\Gamma}_L \Psi_{L,\alpha,+} \Psi_{L,\alpha,+}^{\dagger} \boldsymbol{\Gamma}_L \boldsymbol{G}_{0,N+1}^{A} \boldsymbol{\Gamma}_R \Psi_{R,\gamma,+} \\
&= \sum_{\gamma\alpha} \frac{1}{\hbar v_{R,\gamma}} \Psi_{R,\gamma,+}^{\dagger} \boldsymbol{\Gamma}_R \boldsymbol{G}_{N+1,0}^{R} \boldsymbol{\Gamma}_L \Psi_{L,\alpha,+} \frac{1}{\hbar v_{\alpha,L}} \Psi_{L,\alpha,+}^{\dagger} \boldsymbol{\Gamma}_L \boldsymbol{G}_{0,N+1}^{A} \boldsymbol{\Gamma}_R \Psi_{R,\gamma,+} \\
&= \operatorname{tr}\left[\boldsymbol{\Gamma}_R \boldsymbol{\Psi}_{R,+} \boldsymbol{V}_R^{-1} \boldsymbol{\Psi}_{R,+}^{\dagger} \boldsymbol{\Gamma}_R \boldsymbol{G}_{N+1,0}^{R} \boldsymbol{\Gamma}_L \boldsymbol{\Psi}_{L,+} \boldsymbol{V}_L^{-1} \boldsymbol{\Psi}_{L,+}^{\dagger} \boldsymbol{\Gamma}_L \boldsymbol{G}_{0,N+1}^{A} \right]
\end{aligned}$$

Como

$$\boldsymbol{\Gamma}_R^{-1} = \frac{1}{\hbar} \boldsymbol{\Psi}_R \cdot \boldsymbol{V}^{-1} \cdot \boldsymbol{\Psi}_R^{\dagger}.$$

obtemos

$$\mathcal{T}(E) = \sum_{\gamma\alpha} \frac{v_{\gamma,R}}{v_{\alpha,L}} \left| t_{\gamma\alpha}^{R\leftarrow L} \right|^2 = \operatorname{tr}\left[\boldsymbol{\Gamma}_R \boldsymbol{G}_{N+1,0}^{R} \boldsymbol{\Gamma}_L \boldsymbol{G}_{0,N+1}^{A} \right]$$

Formula de Caroli.

3 Derivação heurística da formula de Caroli

A fórmula de Caroli pode ser derivada de uma forma alternativa. Nesta derivação, fazemos as mesmas suposições que na deviração da fórmula de Landauer-Büttiker:

(i) A corrente é devido ao desiquilíbrio entre a ocupação dos estalhos de espalhamento que se propagam para a direita e esquerda;

(ii) a ocupação dos estados que se propagam para a direita (esquerda) é controlada pelo potencial químico do contacto esquerdo (direito).

A diferença nesta derivação é na forma como os estados de espalhamento são construidos. Em vez de os contruirmos a partir de estados propagantes, agora os estados de espalhamento vão ser construidos a partir dos estados dos contactos isolados.

3.1 Estados de espalhamento e equação de Lippmann-Schwinger

Mais uma vez, vamos separar o sistema em 3 partes, de tal forma que

$$H = \begin{bmatrix} \boldsymbol{H}_R & \boldsymbol{V}_{R,C} & 0 \\ \boldsymbol{V}_{C,R} & \boldsymbol{H}_C & \boldsymbol{V}_{C,L} \\ 0 & \boldsymbol{V}_{L,C} & \boldsymbol{H}_L \end{bmatrix}.$$

Estados de espalhamento do sistema inteiro, obdecem à equação

$$\begin{bmatrix} E - \boldsymbol{H}_R & 0 & 0 \\ 0 & E - \boldsymbol{H}_C & 0 \\ 0 & 0 & E - \boldsymbol{H}_L \end{bmatrix} \begin{bmatrix} \Psi_L \\ \Psi_C \\ \Psi_R \end{bmatrix} = \begin{bmatrix} 0 & \boldsymbol{V}_{R,C} & 0 \\ \boldsymbol{V}_{C,R} & 0 & \boldsymbol{V}_{C,L} \\ 0 & \boldsymbol{V}_{L,C} & 0 \end{bmatrix} \begin{bmatrix} \Psi_L \\ \Psi_C \\ \Psi_R \end{bmatrix}.$$

Esta equação tem solução formal dada pela equação de Lippmann-Schwinger:

$$\begin{bmatrix} \Psi_L \\ \Psi_C \\ \Psi_R \end{bmatrix} = \begin{bmatrix} \Phi_L \\ \Phi_C \\ \Phi_R \end{bmatrix} + \begin{bmatrix} \boldsymbol{g}_{L,L}^R(E) & 0 & 0 \\ 0 & \boldsymbol{g}_{C,C}^R(E) & 0 \\ 0 & 0 & \boldsymbol{g}_{R,R}^R(E) \end{bmatrix} \begin{bmatrix} 0 & \boldsymbol{V}_{R,C} & 0 \\ \boldsymbol{V}_{C,R} & 0 & \boldsymbol{V}_{C,L} \\ 0 & \boldsymbol{V}_{L,C} & 0 \end{bmatrix} \begin{bmatrix} \Psi_L \\ \Psi_C \\ \Psi_R \end{bmatrix}.$$

onde $\boldsymbol{g}_{i,i}^R(E) = \left[E + i0^+ - \boldsymbol{H}_i\right]^{-1}$ e

$$\begin{bmatrix} E - \boldsymbol{H}_R & 0 & 0 \\ 0 & E - \boldsymbol{H}_C & 0 \\ 0 & 0 & E - \boldsymbol{H}_L \end{bmatrix} \begin{bmatrix} \Phi_L \\ \Phi_C \\ \Phi_R \end{bmatrix} = 0$$

é uma solução particular do sistema não perturbado (sem contactos ligados), $(E - \boldsymbol{H}_0)\,\Phi^0 = 0$. De forma mais compacta, escrevendo

$$\boldsymbol{H} = \boldsymbol{H}_0 + \boldsymbol{V}$$
$$\boldsymbol{H}_0 = \begin{bmatrix} \boldsymbol{H}_R & 0 & 0 \\ 0 & \boldsymbol{H}_C & 0 \\ 0 & 0 & \boldsymbol{H}_L \end{bmatrix}$$
$$\boldsymbol{V} = \begin{bmatrix} 0 & \boldsymbol{V}_{R,C} & 0 \\ \boldsymbol{V}_{C,R} & 0 & \boldsymbol{V}_{C,L} \\ 0 & \boldsymbol{V}_{L,C} & 0 \end{bmatrix}$$

temos

$$[E - \boldsymbol{H}_0 - \boldsymbol{V}]\,\Psi = 0 \Leftrightarrow [E - \boldsymbol{H}_0]\,\Psi = \boldsymbol{V}\Psi \Rightarrow \Psi = \Phi + \boldsymbol{g}^R \boldsymbol{V}\Psi.$$

Definindo o operador resolvente/função de Green retardada completa como

$$\left[E + i0^+ - \boldsymbol{H}_0 - \boldsymbol{V}\right] \boldsymbol{G}^R = \mathbf{1} \Leftrightarrow \boldsymbol{G}^R = \boldsymbol{g}^R + \boldsymbol{g}^R \boldsymbol{V} \boldsymbol{G}^R.$$
$$\boldsymbol{G}^R \left[E + i0^+ - \boldsymbol{H}_0 - \boldsymbol{V}\right] = \mathbf{1} \Leftrightarrow \boldsymbol{G}^R = \boldsymbol{g}^R + \boldsymbol{G}^R \boldsymbol{V} \boldsymbol{g}^R$$

Podemos escrever

$$\Psi = \Phi + \boldsymbol{G}^R \boldsymbol{V}\Phi.$$

De forma mais explicita, temos

$$\begin{bmatrix} \Psi_L \\ \Psi_C \\ \Psi_R \end{bmatrix} = \begin{bmatrix} \Phi_L \\ \Phi_C \\ \Phi_R \end{bmatrix} + \begin{bmatrix} \boldsymbol{G}^R_{L,L}(E) & \boldsymbol{G}^R_{L,C}(E) & \boldsymbol{G}^R_{L,R}(E) \\ \boldsymbol{G}^R_{C,L}(E) & \boldsymbol{G}^R_{C,C}(E) & \boldsymbol{G}^R_{C,R}(E) \\ \boldsymbol{G}^R_{R,L}(E) & \boldsymbol{G}^R_{R,C}(E) & \boldsymbol{G}^R_{R,R}(E) \end{bmatrix} \begin{bmatrix} 0 & \boldsymbol{V}_{R,C} & 0 \\ \boldsymbol{V}_{C,R} & 0 & \boldsymbol{V}_{C,L} \\ 0 & \boldsymbol{V}_{L,C} & 0 \end{bmatrix} \begin{bmatrix} \Phi_L \\ \Phi_C \\ \Phi_R \end{bmatrix}.$$

Podemos pensar num estado estacionário do contacto L como sendo a sobreposição de estados que se propagam da esquerda para a direita e que são reflectidos na extremidade do contacto. Assim que os contactos são ligados, este estado transforma-se num estado espalhado. Logo um estado espalhado que se propaga da esquerda para a direita pode ser escrito como

$$\begin{aligned} \begin{bmatrix} \Psi^+_{L,\alpha} \\ \Psi^+_{C,\alpha} \\ \Psi^+_{R,\alpha} \end{bmatrix} &= \begin{bmatrix} \Phi_{L,\alpha} \\ 0 \\ 0 \end{bmatrix} + \begin{bmatrix} \boldsymbol{G}^R_{L,L}(E) & \boldsymbol{G}^R_{L,C}(E) & \boldsymbol{G}^R_{L,R}(E) \\ \boldsymbol{G}^R_{C,L}(E) & \boldsymbol{G}^R_{C,C}(E) & \boldsymbol{G}^R_{C,R}(E) \\ \boldsymbol{G}^R_{R,L}(E) & \boldsymbol{G}^R_{R,C}(E) & \boldsymbol{G}^R_{R,R}(E) \end{bmatrix} \begin{bmatrix} 0 & \boldsymbol{V}_{R,C} & 0 \\ \boldsymbol{V}_{C,R} & 0 & \boldsymbol{V}_{C,L} \\ 0 & \boldsymbol{V}_{L,C} & 0 \end{bmatrix} \begin{bmatrix} \Phi_{L,\alpha} \\ 0 \\ 0 \end{bmatrix} \\ &= \begin{bmatrix} \Phi_{L,\alpha} + \boldsymbol{G}^R_{L,C}(E)\boldsymbol{V}_{C,L}\Phi_{L,\alpha} \\ \boldsymbol{G}^R_{C,C}(E)\boldsymbol{V}_{C,L}\Phi_{L,\alpha} \\ \boldsymbol{G}^R_{R,C}(E)\boldsymbol{V}_{C,L}\Phi_{L,\alpha} \end{bmatrix} \end{aligned}$$

De igual forma, um estado que se propaga da direita para a esquerda, pode ser construido a partir de

$$\begin{aligned} \begin{bmatrix} \Psi^-_{L,\gamma} \\ \Psi^-_{C,\gamma} \\ \Psi^-_{R,\gamma} \end{bmatrix} &= \begin{bmatrix} 0 \\ 0 \\ \Phi_{R,\gamma} \end{bmatrix} + \begin{bmatrix} \boldsymbol{G}^R_{L,L}(E) & \boldsymbol{G}^R_{L,C}(E) & \boldsymbol{G}^R_{L,R}(E) \\ \boldsymbol{G}^R_{C,L}(E) & \boldsymbol{G}^R_{C,C}(E) & \boldsymbol{G}^R_{C,R}(E) \\ \boldsymbol{G}^R_{R,L}(E) & \boldsymbol{G}^R_{R,C}(E) & \boldsymbol{G}^R_{R,R}(E) \end{bmatrix} \begin{bmatrix} 0 & \boldsymbol{V}_{R,C} & 0 \\ \boldsymbol{V}_{C,R} & 0 & \boldsymbol{V}_{C,L} \\ 0 & \boldsymbol{V}_{L,C} & 0 \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ \Phi_{R,\gamma} \end{bmatrix} \\ &= \begin{bmatrix} \boldsymbol{G}^R_{L,C}(E)\boldsymbol{V}_{C,R}\Phi_{R,\gamma} \\ \boldsymbol{G}^R_{C,C}(E)\boldsymbol{V}_{C,R}\Phi_{R,\gamma} \\ \Phi_{R,\gamma} + \boldsymbol{G}^R_{R,C}(E)\boldsymbol{V}_{C,R}\Phi_{R,\gamma} \end{bmatrix} \end{aligned}$$

A partir da esquação de Dyson para $\boldsymbol{G}^R$:

$$\begin{aligned} \begin{bmatrix} \boldsymbol{G}^R_{L,L}(E) & \boldsymbol{G}^R_{L,C}(E) & \boldsymbol{G}^R_{L,R}(E) \\ \boldsymbol{G}^R_{C,L}(E) & \boldsymbol{G}^R_{C,C}(E) & \boldsymbol{G}^R_{C,R}(E) \\ \boldsymbol{G}^R_{R,L}(E) & \boldsymbol{G}^R_{R,C}(E) & \boldsymbol{G}^R_{R,R}(E) \end{bmatrix} &= \begin{bmatrix} \boldsymbol{g}^R_{L,L}(E) & 0 & 0 \\ 0 & \boldsymbol{g}^R_{C,C}(E) & 0 \\ 0 & 0 & \boldsymbol{g}^R_{R,R}(E) \end{bmatrix} + \\ &+ \begin{bmatrix} \boldsymbol{g}^R_{L,L}(E) & 0 & 0 \\ 0 & \boldsymbol{g}^R_{C,C}(E) & 0 \\ 0 & 0 & \boldsymbol{g}^R_{R,R}(E) \end{bmatrix} \begin{bmatrix} 0 & \boldsymbol{V}_{R,C} & 0 \\ \boldsymbol{V}_{C,R} & 0 & \boldsymbol{V}_{C,L} \\ 0 & \boldsymbol{V}_{L,C} & 0 \end{bmatrix} \begin{bmatrix} \boldsymbol{G}^R_{L,L}(E) & \boldsymbol{G}^R_{L,C}(E) & \boldsymbol{G}^R_{L,R}(E) \\ \boldsymbol{G}^R_{C,L}(E) & \boldsymbol{G}^R_{C,C}(E) & \boldsymbol{G}^R_{C,R}(E) \\ \boldsymbol{G}^R_{R,L}(E) & \boldsymbol{G}^R_{R,C}(E) & \boldsymbol{G}^R_{R,R}(E) \end{bmatrix} \end{aligned}$$

e da forma alternativa

$$\begin{bmatrix} \boldsymbol{G}^R_{L,L}(E) & \boldsymbol{G}^R_{L,C}(E) & \boldsymbol{G}^R_{L,R}(E) \\ \boldsymbol{G}^R_{C,L}(E) & \boldsymbol{G}^R_{C,C}(E) & \boldsymbol{G}^R_{C,R}(E) \\ \boldsymbol{G}^R_{R,L}(E) & \boldsymbol{G}^R_{R,C}(E) & \boldsymbol{G}^R_{R,R}(E) \end{bmatrix} = \begin{bmatrix} \boldsymbol{g}^R_{L,L}(E) & 0 & 0 \\ 0 & \boldsymbol{g}^R_{C,C}(E) & 0 \\ 0 & 0 & \boldsymbol{g}^R_{R,R}(E) \end{bmatrix} +$$
$$+ \begin{bmatrix} \boldsymbol{G}^R_{L,L}(E) & \boldsymbol{G}^R_{L,C}(E) & \boldsymbol{G}^R_{L,R}(E) \\ \boldsymbol{G}^R_{C,L}(E) & \boldsymbol{G}^R_{C,C}(E) & \boldsymbol{G}^R_{C,R}(E) \\ \boldsymbol{G}^R_{R,L}(E) & \boldsymbol{G}^R_{R,C}(E) & \boldsymbol{G}^R_{R,R}(E) \end{bmatrix} \begin{bmatrix} 0 & \boldsymbol{V}_{R,C} & 0 \\ \boldsymbol{V}_{C,R} & 0 & \boldsymbol{V}_{C,L} \\ 0 & \boldsymbol{V}_{L,C} & 0 \end{bmatrix} \begin{bmatrix} \boldsymbol{g}^R_{L,L}(E) & 0 & 0 \\ 0 & \boldsymbol{g}^R_{C,C}(E) & 0 \\ 0 & 0 & \boldsymbol{g}^R_{R,R}(E) \end{bmatrix}$$

temos que

$$\boldsymbol{G}^R_{L,C}(E) = \boldsymbol{g}^R_{L,L}(E)\boldsymbol{V}_{L,C}\boldsymbol{G}^R_{C,C}(E)$$
$$\boldsymbol{G}^R_{R,C}(E) = \boldsymbol{g}^R_{R,R}(E)\boldsymbol{V}_{R,C}\boldsymbol{G}^R_{C,C}(E)$$

de tal forma que

$$\begin{bmatrix} \Psi^+_{L,\alpha} \\ \Psi^+_{C,\alpha} \\ \Psi^+_{R,\alpha} \end{bmatrix} = \begin{bmatrix} \Phi_{L,\alpha} + \boldsymbol{g}^R_{L,L}(E)\boldsymbol{V}_{L,C}\boldsymbol{G}^R_{C,C}(E)\boldsymbol{V}_{C,L}\Phi_{L,\alpha} \\ \boldsymbol{G}^R_{C,C}(E)\boldsymbol{V}_{C,L}\Phi_{L,\alpha} \\ \boldsymbol{g}^R_{R,R}(E)\boldsymbol{V}_{R,C}\boldsymbol{G}^R_{C,C}(E)\boldsymbol{V}_{C,L}\Phi_{L,\alpha} \end{bmatrix},$$
$$\begin{bmatrix} \Psi^-_{L,\gamma} \\ \Psi^-_{C,\gamma} \\ \Psi^-_{R,\gamma} \end{bmatrix} = \begin{bmatrix} \boldsymbol{g}^R_{L,L}(E)\boldsymbol{V}_{L,C}\boldsymbol{G}^R_{C,C}(E)\boldsymbol{V}_{C,R}\Phi_{R,\gamma} \\ \boldsymbol{G}^R_{C,C}(E)\boldsymbol{V}_{C,R}\Phi_{R,\gamma} \\ \Phi_{R,\gamma} + \boldsymbol{g}^R_{R,R}(E)\boldsymbol{V}_{R,C}\boldsymbol{G}^R_{C,C}(E)\boldsymbol{V}_{C,R}\Phi_{R,\gamma} \end{bmatrix}.$$

3.2 Valor esperado do operador corrente

Estamos agora em posição de calcular a corrente. O operador corrente entre a região central e o contacto direito é dado por

$$\begin{aligned} I = I_{C\to R} &= \frac{dN_R}{dt} \\ &= \frac{i}{\hbar}\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & \boldsymbol{V}_{C,R} \\ 0 & -\boldsymbol{V}_{R,C} & 0 \end{bmatrix}. \end{aligned}$$

Vamos agora calcular a corrente devido a um estado que se propaga da esquerda para a direita, $|\Psi^+_\alpha\rangle$. Obtemos:

$$\begin{aligned} \left\langle \Psi^+_\alpha \right| I \left| \Psi^+_\alpha \right\rangle &= \frac{i}{\hbar}\left(\Psi^\dagger_{C,\alpha,+}\boldsymbol{V}_{C,R}\Psi_{R,\alpha,+} - \Psi^\dagger_{R,\alpha,+}\boldsymbol{V}_{R,C}\Psi_{C,\alpha,+}\right) \\ &= \frac{i}{\hbar}\Phi^\dagger_{L,\alpha}\boldsymbol{V}_{L,C}\boldsymbol{G}^A_{C,C}(E)\boldsymbol{V}_{C,R}\boldsymbol{g}^R_{R,R}(E)\boldsymbol{V}_{R,C}\boldsymbol{G}^R_{C,C}(E)\boldsymbol{V}_{C,L}\Phi_{L,\alpha} \\ &- \frac{i}{\hbar}\Phi^\dagger_{L,\alpha}\boldsymbol{V}_{L,C}\boldsymbol{G}^A_{C,C}(E)\boldsymbol{V}_{C,R}\boldsymbol{g}^A_{R,R}(E)\boldsymbol{V}_{R,C}\boldsymbol{G}^R_{C,C}(E)\boldsymbol{V}_{C,L}\Phi_{L,\alpha} \end{aligned}$$

onde $\boldsymbol{G}^A = \left[\boldsymbol{G}^R\right]^\dagger$ e $\boldsymbol{g}^A = \left[\boldsymbol{g}^R\right]^\dagger$. Definindo as auto-energias como

$$\boldsymbol{\Sigma}^{R/A}_L(E) = \boldsymbol{V}_{C,L}\boldsymbol{g}^{R/A}_{L,L}(E)\boldsymbol{V}_{L,C}$$
$$\boldsymbol{\Sigma}^{R/A}_R(E) = \boldsymbol{V}_{C,R}\boldsymbol{g}^{R/A}_{R,R}(E)\boldsymbol{V}_{L,C}.$$

Podemos escrever

$$\left\langle \Psi^+_\alpha \right| I \left| \Psi^+_\alpha \right\rangle = \frac{i}{\hbar}\Phi^\dagger_{L,\alpha}\boldsymbol{V}_{L,C}\boldsymbol{G}^A_{C,C}(E)\left(\boldsymbol{\Sigma}^R_R(E) - \boldsymbol{\Sigma}^A_R(E)\right)\boldsymbol{G}^R_{C,C}(E)\boldsymbol{V}_{C,L}\Phi_{L,\alpha}.$$

Definimos as matrizes $\boldsymbol{\Gamma}$ como

$$\boldsymbol{\Gamma}_L(E) = i\left[\boldsymbol{\Sigma}^R_L(E) - \boldsymbol{\Sigma}^A_L(E)\right]$$
$$\boldsymbol{\Gamma}_R(E) = i\left[\boldsymbol{\Sigma}^R_R(E) - \boldsymbol{\Sigma}^A_R(E)\right]$$

de tal forma que

$$\left\langle \Psi_\alpha^+ \right| I \left| \Psi_\alpha^+ \right\rangle = \frac{1}{\hbar} \Phi_{L,\alpha}^\dagger \boldsymbol{V}_{L,C} \boldsymbol{G}_{C,C}^A(E) \boldsymbol{\Gamma}_R(E) \boldsymbol{G}_{C,C}^R(E) \boldsymbol{V}_{C,L} \Phi_{L,\alpha}.$$

A corrente devido a estados que se propagam da esquerda para a direita é então

$$\begin{aligned}
I_+ &= \sum_\alpha f_L(\epsilon_\alpha) \left\langle \Psi_\alpha^+ \right| I \left| \Psi_\alpha^+ \right\rangle \\
&= \int dE f_L(E) \sum_\alpha \delta(E-\epsilon_\alpha) \left\langle \Psi_\alpha^+ \right| I \left| \Psi_\alpha^+ \right\rangle \\
&= \frac{1}{\hbar} \int dE f_L(E) \sum_\alpha \delta(E-\epsilon_\alpha) \Phi_{L,\alpha}^\dagger \boldsymbol{V}_{L,C} \boldsymbol{G}_{C,C}^A(E) \boldsymbol{\Gamma}_R(E) \boldsymbol{G}_{C,C}^R(E) \boldsymbol{V}_{C,L} \Phi_{L,\alpha} \\
&= \frac{1}{\hbar} \int dE f_L(E) \mathrm{Tr} \left[\boldsymbol{\Gamma}_R(E) \boldsymbol{G}_{C,C}^R(E) \boldsymbol{V}_{C,L} \left(\sum_\alpha \Phi_{L,\alpha} \Phi_{L,\alpha}^\dagger \delta(E-\epsilon_\alpha) \right) \boldsymbol{V}_{L,C} \boldsymbol{G}_{C,C}^A(E) \right]
\end{aligned}$$

A partir de

$$\boldsymbol{g}_L^{R/A}(E) = \left[E \pm i0^+ - \boldsymbol{H}_L \right]^{-1} = \sum_\alpha \Phi_{L,\alpha} \frac{1}{E \pm i0^+ - \epsilon_\alpha} \Phi_{L,\alpha}^\dagger,$$

(recordar que no sentido de distribuições: $1/(x+i0^+) = P1/x - i\pi\delta(x)$) é fácil de ver que

$$i \left[\boldsymbol{g}^R(E) - \boldsymbol{g}^A(E) \right] = \sum_\alpha \Phi_{L,\alpha} \Phi_{L,\alpha}^\dagger 2\pi \delta(E-\epsilon_\alpha).$$

Logo

$$\sum_\alpha \Phi_{L,\alpha} \Phi_{L,\alpha}^\dagger \delta(E-\epsilon_\alpha) = 2\pi \boldsymbol{\Gamma}_L(E).$$

Temos então que

$$I_+ = \frac{1}{\hbar} \int \frac{dE}{2\pi} f_L(E) \mathrm{Tr} \left[\boldsymbol{\Gamma}_R(E) \boldsymbol{G}_{C,C}^R(E) \boldsymbol{\Gamma}_L(E) \boldsymbol{G}_{C,C}^A(E) \right].$$

Falta agora calcular a corrente devido aos estados que se propagam da direita para a esquerda. Temos então

$$\begin{aligned}
\left\langle \Psi_\gamma^- \right| I \left| \Psi_\gamma^- \right\rangle &= \frac{i}{\hbar} \left(\Psi_{C,\gamma,-}^\dagger \boldsymbol{V}_{C,R} \Psi_{R,\gamma,-} - \Psi_{R,\alpha,+}^\dagger \boldsymbol{V}_{R,C} \Psi_{C,\gamma,-} \right) \\
&= \frac{i}{\hbar} \Phi_{R,\gamma}^\dagger \boldsymbol{V}_{R,C} \boldsymbol{G}_{C,C}^A(E) \boldsymbol{V}_{C,R} \left(\Phi_{R,\gamma} + \boldsymbol{g}_{R,R}^R(E) \boldsymbol{V}_{R,C} \boldsymbol{G}_{C,C}^R(E) \boldsymbol{V}_{C,R} \Phi_{R,\gamma} \right) \\
&- \frac{i}{\hbar} \left(\Phi_{R,\gamma}^\dagger + \Phi_{R,\gamma}^\dagger \boldsymbol{V}_{R,C} \boldsymbol{G}_{C,C}^A(E) \boldsymbol{V}_{C,R} \boldsymbol{g}_{R,R}^A(E) \right) \boldsymbol{V}_{R,C} \boldsymbol{G}_{C,C}^R(E) \boldsymbol{V}_{C,R} \Phi_{R,\gamma} \\
&= \frac{i}{\hbar} \Phi_{R,\gamma}^\dagger \boldsymbol{V}_{R,C} \boldsymbol{G}_{C,C}^A(E) \boldsymbol{V}_{C,R} \Phi_{R,\gamma} + \frac{i}{\hbar} \Phi_{R,\gamma}^\dagger \boldsymbol{V}_{R,C} \boldsymbol{G}_{C,C}^A(E) \boldsymbol{V}_{C,R} \boldsymbol{g}_{R,R}^R(E) \boldsymbol{V}_{R,C} \boldsymbol{G}_{C,C}^R(E) \boldsymbol{V}_{C,R} \Phi_{R,\gamma} \\
&- \frac{i}{\hbar} \Phi_{R,\gamma}^\dagger \boldsymbol{V}_{R,C} \boldsymbol{G}_{C,C}^R(E) \boldsymbol{V}_{C,R} \Phi_{R,\gamma} - \frac{i}{\hbar} \Phi_{R,\gamma}^\dagger \boldsymbol{V}_{R,C} \boldsymbol{G}_{C,C}^A(E) \boldsymbol{V}_{C,R} \boldsymbol{g}_{R,R}^A(E) \boldsymbol{V}_{R,C} \boldsymbol{G}_{C,C}^R(E) \boldsymbol{V}_{C,R} \Phi_{R,\gamma} \\
&= \frac{i}{\hbar} \Phi_{R,\gamma}^\dagger \boldsymbol{V}_{R,C} \left[\boldsymbol{G}_{C,C}^A(E) - \boldsymbol{G}_{C,C}^R(E) \right] \boldsymbol{V}_{C,R} \Phi_{R,\gamma} \\
&+ \frac{i}{\hbar} \Phi_{R,\gamma}^\dagger \boldsymbol{V}_{R,C} \boldsymbol{G}_{C,C}^A(E) \boldsymbol{V}_{C,R} \left[\boldsymbol{g}_{R,R}^R(E) - \boldsymbol{g}_{R,R}^A(E) \right] \boldsymbol{V}_{R,C} \boldsymbol{G}_{C,C}^R(E) \boldsymbol{V}_{C,R} \Phi_{R,\gamma} \\
&= -\frac{1}{\hbar} \Phi_{R,\gamma}^\dagger \boldsymbol{V}_{R,C} \boldsymbol{A}_{C,C}(E) \boldsymbol{V}_{C,R} \Phi_{R,\gamma} + \frac{1}{\hbar} \Phi_{R,\gamma}^\dagger \boldsymbol{V}_{R,C} \boldsymbol{G}_{C,C}^A(E) \boldsymbol{\Gamma}_R(E) \boldsymbol{G}_{C,C}^R(E) \boldsymbol{V}_{C,R} \Phi_{R,\gamma}.
\end{aligned}$$

Vamos agora escrever

$$\begin{aligned}
\boldsymbol{G}_{C,C}^A(E) \boldsymbol{\Gamma}_R(E) \boldsymbol{G}_{C,C}^R(E) &= \boldsymbol{G}_{C,C}^A(E) \left(\boldsymbol{\Gamma}(E) - \boldsymbol{\Gamma}_L(E) \right) \boldsymbol{G}_{C,C}^R(E) \\
&= \boldsymbol{G}_{C,C}^A(E) \boldsymbol{\Gamma}(E) \boldsymbol{G}_{C,C}^R(E) - \boldsymbol{G}_{C,C}^A(E) \boldsymbol{\Gamma}_L(E) \boldsymbol{G}_{C,C}^R(E).
\end{aligned}$$

onde $\boldsymbol{\Gamma}(E) = \boldsymbol{\Gamma}_L(E) + \boldsymbol{\Gamma}_R(E)$. Vamos agora ver que

$$\begin{aligned}
\boldsymbol{A}_{C,C}(E) &= i\left(\boldsymbol{G}^R_{C,C}(E) - \boldsymbol{G}^A_{C,C}(E)\right) \\
&= i\boldsymbol{G}^A_{C,C}(E)\left(\left[\boldsymbol{G}^A_{C,C}(E)\right]^{-1} - \left[\boldsymbol{G}^R_{C,C}(E)\right]^{-1}\right)\boldsymbol{G}^R_{C,C}(E) \\
&= i\boldsymbol{G}^A_{C,C}(E)\left(\left[E - \boldsymbol{H}_C - \boldsymbol{\Sigma}^A(E)\right] - \left[E - \boldsymbol{H}_C - \boldsymbol{\Sigma}^R(E)\right]\right)\boldsymbol{G}^R_{C,C}(E) \\
&= i\boldsymbol{G}^A_{C,C}(E)\left(\boldsymbol{\Sigma}^R(E) - \boldsymbol{\Sigma}^A(E)\right)\boldsymbol{G}^R_{C,C}(E) \\
&= \boldsymbol{G}^A_{C,C}(E)\boldsymbol{\Gamma}(E)\boldsymbol{G}^R_{C,C}(E).
\end{aligned}$$

Usando este resultado podemos escrever

$$\begin{aligned}
\left\langle \Psi^-_\gamma \right| I \left|\Psi^-_\gamma\right\rangle &= -\frac{1}{\hbar}\Phi^\dagger_{R,\gamma}\boldsymbol{V}_{R,C}\boldsymbol{A}_{C,C}(E)\boldsymbol{V}_{C,R}\Phi_{R,\gamma} + \frac{1}{\hbar}\Phi^\dagger_{R,\gamma}\boldsymbol{V}_{R,C}\boldsymbol{G}^A_{C,C}(E)\boldsymbol{\Gamma}(E)\boldsymbol{G}^R_{C,C}(E)\boldsymbol{V}_{C,R}\Phi_{R,\gamma} \\
&\quad - \frac{1}{\hbar}\Phi^\dagger_{R,\gamma}\boldsymbol{V}_{R,C}\boldsymbol{G}^A_{C,C}(E)\boldsymbol{\Gamma}_L(E)\boldsymbol{G}^R_{C,C}(E)\boldsymbol{V}_{C,R}\Phi_{R,\gamma} \\
&= -\frac{1}{\hbar}\Phi^\dagger_{R,\gamma}\boldsymbol{V}_{R,C}\boldsymbol{G}^A_{C,C}(E)\boldsymbol{\Gamma}_L(E)\boldsymbol{G}^R_{C,C}(E)\boldsymbol{V}_{C,R}\Phi_{R,\gamma}
\end{aligned}$$

Somando a contribuição de todos os estados $\left|\Psi^-_\gamma\right\rangle$, obtemos

$$\begin{aligned}
I_- &= \sum_\gamma f_R(\epsilon_\gamma)\left\langle \Psi^-_\gamma \right| I \left|\Psi^-_\gamma\right\rangle \\
&= \int dE f_R(E)\sum_\gamma \delta(E-\epsilon_\gamma)\left\langle \Psi^-_\gamma \right| I \left|\Psi^-_\gamma\right\rangle \\
&= -\frac{1}{\hbar}\int dE f_R(E)\sum_\gamma \delta(E-\epsilon_\gamma)\Phi^\dagger_{R,\gamma}\boldsymbol{V}_{R,C}\boldsymbol{G}^A_{C,C}(E)\boldsymbol{\Gamma}_L(E)\boldsymbol{G}^R_{C,C}(E)\boldsymbol{V}_{C,R}\Phi_{R,\gamma} \\
&= -\frac{1}{\hbar}\int dE f_R(E)\mathrm{Tr}\left[\boldsymbol{V}_{C,R}\sum_\gamma \Phi_{R,\gamma}\Phi^\dagger_{R,\gamma}\delta(E-\epsilon_\gamma)\boldsymbol{V}_{R,C}\boldsymbol{G}^A_{C,C}(E)\boldsymbol{\Gamma}_L(E)\boldsymbol{G}^R_{C,C}(E)\right] \\
&= -\frac{1}{\hbar}\int \frac{dE}{2\pi} f_R(E)\mathrm{Tr}\left[\boldsymbol{\Gamma}_R(E)\boldsymbol{G}^A_{C,C}(E)\boldsymbol{\Gamma}_L(E)\boldsymbol{G}^R_{C,C}(E)\right]
\end{aligned}$$

A corrente total é dada por

$$\begin{aligned}
I_{L\to R} &= I_+ + I_- \\
&= \frac{1}{\hbar}\int \frac{dE}{2\pi} f_L(E)\mathrm{Tr}\left[\boldsymbol{\Gamma}_R(E)\boldsymbol{G}^R_{C,C}(E)\boldsymbol{\Gamma}_L(E)\boldsymbol{G}^A_{C,C}(E)\right] - \frac{1}{\hbar}\int \frac{dE}{2\pi} f_R(E)\mathrm{Tr}\left[\boldsymbol{\Gamma}_R(E)\boldsymbol{G}^A_{C,C}(E)\boldsymbol{\Gamma}_L(E)\boldsymbol{G}^R_{C,C}(E)\right].
\end{aligned}$$

Mais uma vez, se $f_L(E) = f_R(E)$, a corrente deve ser nula, pelo que devemos ter o resultado:

$$\mathrm{Tr}\left[\boldsymbol{\Gamma}_R(E)\boldsymbol{G}^R_{C,C}(E)\boldsymbol{\Gamma}_L(E)\boldsymbol{G}^A_{C,C}(E)\right] = \mathrm{Tr}\left[\boldsymbol{\Gamma}_R(E)\boldsymbol{G}^A_{C,C}(E)\boldsymbol{\Gamma}_L(E)\boldsymbol{G}^R_{C,C}(E)\right]$$

e obtemos

$$I_{L\to R} = \frac{1}{\hbar}\int \frac{dE}{2\pi}\left[f_L(E) - f_R(E)\right]\mathrm{Tr}\left[\boldsymbol{\Gamma}_R(E)\boldsymbol{G}^R_{C,C}(E)\boldsymbol{\Gamma}_L(E)\boldsymbol{G}^A_{C,C}(E)\right].$$

Na realidade, isto ode ser verificado explicitamente. Basta recordar que

$$\boldsymbol{A}_{C,C}(E) = i\left[\boldsymbol{G}^R_{C,C}(E) - \boldsymbol{G}^A_{C,C}(E)\right] = \boldsymbol{G}^A_{C,C}(E)\boldsymbol{\Gamma}(E)\boldsymbol{G}^R_{C,C}(E) = \boldsymbol{G}^R_{C,C}(E)\boldsymbol{\Gamma}(E)\boldsymbol{G}^A_{C,C}(E).$$

Podemos então escrever

$$\begin{aligned}
\mathrm{Tr}\left[\boldsymbol{\Gamma}_R(E)\cdot\boldsymbol{G}^R_{C,C}(E)\cdot\boldsymbol{\Gamma}_L(E)\cdot\boldsymbol{G}^A_{C,C}(E)\right] &= \mathrm{Tr}\left[(\boldsymbol{\Gamma}(E) - \boldsymbol{\Gamma}_L(E))\cdot\boldsymbol{G}^R_{C,C}(E)\cdot(\boldsymbol{\Gamma}(E) - \boldsymbol{\Gamma}_R(E))\cdot\boldsymbol{G}^A_{C,C}(E)\right] \\
&= \mathrm{Tr}\left[\boldsymbol{\Gamma}(E)\cdot\boldsymbol{G}^R_{C,C}(E)\cdot\boldsymbol{\Gamma}(E)\cdot\boldsymbol{G}^A_{C,C}(E)\right] \\
&\quad - \mathrm{Tr}\left[\boldsymbol{\Gamma}(E)\cdot\boldsymbol{G}^R_{C,C}(E)\cdot\boldsymbol{\Gamma}_R(E)\cdot\boldsymbol{G}^A_{C,C}(E)\right] \\
&\quad - \mathrm{Tr}\left[\boldsymbol{\Gamma}_L(E)\cdot\boldsymbol{G}^R_{C,C}(E)\cdot\boldsymbol{\Gamma}(E)\cdot\boldsymbol{G}^A_{C,C}(E)\right] \\
&\quad + \mathrm{Tr}\left[\boldsymbol{\Gamma}_L(E)\cdot\boldsymbol{G}^R_{C,C}(E)\cdot\boldsymbol{\Gamma}_R(E)\cdot\boldsymbol{G}^A_{C,C}(E)\right].
\end{aligned}$$

Escrevendo agora:

$$\operatorname{Tr}\left[\mathbf{\Gamma}(E)\cdot\boldsymbol{G}^R_{C,C}(E)\cdot\mathbf{\Gamma}(E)\cdot\boldsymbol{G}^A_{C,C}(E)\right]=\operatorname{Tr}\left[\mathbf{\Gamma}(E)\cdot\boldsymbol{A}_{C,C}(E)\right]$$

e

$$\begin{aligned}
&\operatorname{Tr}\left[\mathbf{\Gamma}(E)\cdot\boldsymbol{G}^R_{C,C}(E)\cdot\mathbf{\Gamma}_R(E)\cdot\boldsymbol{G}^A_{C,C}(E)\right]+\operatorname{Tr}\left[\mathbf{\Gamma}_L(E)\cdot\boldsymbol{G}^R_{C,C}(E)\cdot\mathbf{\Gamma}(E)\cdot\boldsymbol{G}^A_{C,C}(E)\right]=\\
&=\operatorname{Tr}\left[\mathbf{\Gamma}_R(E)\cdot\boldsymbol{G}^A_{C,C}(E)\cdot\mathbf{\Gamma}(E)\cdot\boldsymbol{G}^R_{C,C}(E)\right]+\operatorname{Tr}\left[\mathbf{\Gamma}_L(E)\cdot\boldsymbol{G}^R_{C,C}(E)\cdot\mathbf{\Gamma}(E)\cdot\boldsymbol{G}^A_{C,C}(E)\right]\\
&=\operatorname{Tr}\left[(\mathbf{\Gamma}_R(E)+\mathbf{\Gamma}_L(E))\cdot\boldsymbol{A}_{C,C}(E)\right]\\
&=\operatorname{Tr}\left[\mathbf{\Gamma}(E)\cdot\boldsymbol{A}_{C,C}(E)\right]
\end{aligned}$$

concluímos que

$$\operatorname{Tr}\left[\mathbf{\Gamma}_R(E)\cdot\boldsymbol{G}^R_{C,C}(E)\cdot\mathbf{\Gamma}_L(E)\cdot\boldsymbol{G}^A_{C,C}(E)\right]=\operatorname{Tr}\left[\mathbf{\Gamma}_L(E)\cdot\boldsymbol{G}^R_{C,C}(E)\cdot\mathbf{\Gamma}_R(E)\cdot\boldsymbol{G}^A_{C,C}(E)\right].$$

4 Comparação entre fórmula de Landauer-Büttiker e fórmula de Caroli

Nas duas secções anteriores, mostramos que a corrente num sistema mesoscópico pode ser escrita na forma

$$I_{L\to R}=\frac{1}{\hbar}\int\frac{dE}{2\pi}\left[f_L(E)-f_R(E)\right]\operatorname{Tr}\left[\mathbf{\Gamma}_R(E)\boldsymbol{G}^R_{C,C}(E)\mathbf{\Gamma}_L(E)\boldsymbol{G}^A_{C,C}(E)\right]$$

onde

$$\begin{aligned}
\boldsymbol{G}^R_{C,C}(E)&=\left[E-\boldsymbol{H}_C-\mathbf{\Sigma}^R_L(E)-\mathbf{\Sigma}^R_R(E)\right]^{-1}\\
\mathbf{\Gamma}_L(E)&=i\left[\mathbf{\Sigma}^R_L(E)-\mathbf{\Sigma}^A_L(E)\right]\\
\mathbf{\Gamma}_R(E)&=i\left[\mathbf{\Sigma}^R_R(E)-\mathbf{\Sigma}^A_R(E)\right]
\end{aligned}$$

No entanto o significado de $\mathbf{\Sigma}_{L/R}(E)$ é aparentemente, muito distinto.

Na derivação da fórmula de Landauer:

$$\begin{aligned}
\mathbf{\Sigma}^R_L&\underset{LB}{=}\boldsymbol{v}^\dagger_L\cdot\mathbf{\Psi}_{L,-}\cdot\mathbf{\Lambda}^{-1}_{L,-}\cdot\mathbf{\Psi}^{-1}_{L,-}\\
\mathbf{\Sigma}^A_L&\underset{LB}{=}\boldsymbol{v}^\dagger_L\cdot\mathbf{\Psi}_{L,+}\cdot\mathbf{\Lambda}^{-1}_{L,+}\cdot\mathbf{\Psi}^{-1}_{L,+}\\
\mathbf{\Sigma}^R_R&\underset{LB}{=}\boldsymbol{v}_R\cdot\mathbf{\Psi}_{R,+}\cdot\mathbf{\Lambda}_{R,+}\cdot\mathbf{\Psi}^{-1}_{R,+}\\
\mathbf{\Sigma}^A_R&\underset{LB}{=}\boldsymbol{v}_R\cdot\mathbf{\Psi}_{R,-}\cdot\mathbf{\Lambda}_{R,-}\cdot\mathbf{\Psi}^{-1}_{R,-}
\end{aligned}$$

enquanto que na fórmula de Caroli, as auto-energias são dadas por

$$\begin{aligned}
\mathbf{\Sigma}^R_L&\underset{C}{=}\boldsymbol{V}_{C,L}\cdot\boldsymbol{g}^R_{L,L}\cdot\boldsymbol{V}_{L,C}\\
\mathbf{\Sigma}^A_L&\underset{C}{=}\boldsymbol{V}_{C,L}\cdot\boldsymbol{g}^A_{L,L}\cdot\boldsymbol{V}_{L,C}\\
\mathbf{\Sigma}^R_R&\underset{C}{=}\boldsymbol{V}_{C,R}\cdot\boldsymbol{g}^R_{R,R}\cdot\boldsymbol{V}_{R,C}\\
\mathbf{\Sigma}^A_L&\underset{C}{=}\boldsymbol{V}_{C,R}\cdot\boldsymbol{g}^A_{R,R}\cdot\boldsymbol{V}_{R,C}.
\end{aligned}$$

Como podem estes resultados ser reconciliados?

A resposta é obtida se tentarmos calcular $\boldsymbol{g}^R_{L,L}$ quando o contacto é semi-intinito e invariante de translação. $\boldsymbol{g}^R_{L,L}$ é então solução de

$$\begin{bmatrix}\ddots&\ddots&\\ \ddots&E-\boldsymbol{h}_L&-\boldsymbol{v}_L\\ &-\boldsymbol{v}^\dagger_L&E-\boldsymbol{h}_L\end{bmatrix}\begin{bmatrix}\ddots&\ddots&\vdots\\ \ddots&\boldsymbol{g}^R_{-2,-2}&\boldsymbol{g}^R_{-2,-1}\\ \cdots&\boldsymbol{g}^R_{-1,-2}&\boldsymbol{g}^R_{-1,-1}\end{bmatrix}=\begin{bmatrix}\ddots&\ddots&\vdots\\ \ddots&1&0\\ \cdots&0&1\end{bmatrix}.$$

Vamos focarnos a coluna $\boldsymbol{g}^R_{n,-1}$. Temos então que

$$\begin{bmatrix} \ddots & \ddots & \\ \ddots & E-\boldsymbol{h}_L & -\boldsymbol{v}_L \\ & -\boldsymbol{v}_L^\dagger & E-\boldsymbol{h}_L \end{bmatrix} \begin{bmatrix} \vdots \\ \boldsymbol{g}^R_{-2,-1} \\ \boldsymbol{g}^R_{-1,-1} \end{bmatrix} = \begin{bmatrix} \vdots \\ 0 \\ 1 \end{bmatrix}.$$

Para $n < -1$, temos a equação

$$-\boldsymbol{v}_L^\dagger \boldsymbol{g}^R_{n-1,-1} + (E-\boldsymbol{h}_L)\,\boldsymbol{g}^R_{n,-1} - \boldsymbol{v}_L \boldsymbol{g}^R_{n+1,-1} = 0.$$

Nós sabemos que estados propagantes satisfazem a equação:

$$\boldsymbol{v}_L^\dagger \Psi_{\alpha,-,n-1} + (E-\boldsymbol{h}_L)\,\Psi_{\alpha,-,n} - \boldsymbol{v}_L \Psi_{\alpha,-,n+1} = 0.$$

Podemos então procurar uma soluãço para $\boldsymbol{g}^R_{n,-1}$ expandindo a função de Green em termos de estados propagantes:

$$\boldsymbol{g}^R_{n,-1} = \sum_\alpha \Psi_{\alpha,-,n} U_\alpha = \sum_\alpha \lambda^{n+1}_{\alpha,-} \Psi_{\alpha,-,-1} U_\alpha,$$

onde U_α são um conjunto de vectores linhas, cuja forma temos de encontrar. A razão para usarmos os estados Ψ_- e não os estados Ψ_+ está relacionado com as propriedades da funções de Green retardadas. Estas descrevem respostas causais, isto é, $\boldsymbol{g}^R_{n,-1}$ descreve a resposta causal no sítio n devido a uma perturbação no sítio -1. Como tal $\boldsymbol{g}^R_{n,-1}$ deve ser uma onda que se propaga de $-1 \to n$ (com $n < -1$) e portanto é do tipo Ψ_-. A equação para $n = -1$ é:

$$-\boldsymbol{v}_L^\dagger \boldsymbol{g}^R_{-2,-1} + (E-\boldsymbol{h}_L)\,\boldsymbol{g}^R_{-1,-1} = \boldsymbol{1}$$

O que podemos escrever como

$$\begin{aligned} -\boldsymbol{v}_L^\dagger \boldsymbol{g}^R_{-2,-1} + (E-\boldsymbol{h}_L)\,\boldsymbol{g}^R_{-1,-1} &= \sum_\alpha \Big(-\boldsymbol{v}_L^\dagger \Psi_{\alpha,-,-2} U_\alpha + (E-\boldsymbol{h}_L)\,\Psi_{\alpha,-,-1} U_\alpha - \boldsymbol{v}_L \Psi_{\alpha,-,0} U_\alpha + \boldsymbol{v}_L \Psi_{\alpha,-,0} U_\alpha \Big) \\ &= \sum_\alpha \Big(-\boldsymbol{v}_L^\dagger \Psi_{\alpha,-,-2} + (E-\boldsymbol{h}_L)\,\Psi_{\alpha,-,-1} - \boldsymbol{v}_L \Psi_{\alpha,-,0} \Big) U_\alpha + \sum_\alpha \left(\boldsymbol{v}_L \Psi_{\alpha,-,0} U_\alpha \right) \\ &= \boldsymbol{v}_L \boldsymbol{\Psi}_- \cdot \boldsymbol{U}. \end{aligned}$$

Temos então que

$$\boldsymbol{v}_L \boldsymbol{\Psi}_- \cdot \boldsymbol{U} = \boldsymbol{1}.$$

Resolvendo em ordem a $\boldsymbol{U}$, obtemos

$$\boldsymbol{U} = \boldsymbol{\Psi}_-^{-1} \cdot \boldsymbol{v}_L^{-1}.$$

Logo:

$$\begin{aligned} \boldsymbol{g}^R_{-1,-1} &= \sum_\alpha \Psi_{\alpha,-,-1} U_\alpha \\ &= \sum_\alpha \Psi_{\alpha,-,0} \lambda^{-1}_{\alpha,-} U_\alpha \\ &= \boldsymbol{\Psi}_- \cdot \boldsymbol{\Lambda}_-^{-1} \cdot \boldsymbol{U} \\ &= \boldsymbol{\Psi}_- \cdot \boldsymbol{\Lambda}_-^{-1} \cdot \boldsymbol{\Psi}_-^{-1} \cdot \boldsymbol{v}_L^{-1}. \end{aligned}$$

Repondo os indices que identificam o contacto, a auto-energia é então dada por

$$\begin{aligned} \boldsymbol{\Sigma}^R_L &\underset{C}{=} \boldsymbol{V}_{C,L} \cdot \boldsymbol{g}^R_{L,L} \cdot \boldsymbol{V}_{L,C} \\ &= \boldsymbol{v}_{0,-1} \cdot \boldsymbol{g}^R_{L,-1;L,-1} \cdot \boldsymbol{v}_{-1,0} \\ &= \boldsymbol{v}_L^\dagger \cdot \boldsymbol{g}^R_{L,-1;L,-1} \cdot \boldsymbol{v}_L \\ &= \boldsymbol{v}_L^\dagger \cdot \boldsymbol{\Psi}_{L,-} \cdot \boldsymbol{\Lambda}^{-1}_{L,-} \cdot \boldsymbol{\Psi}^{-1}_{L,-}, \end{aligned}$$

o que está em concordância com o obtido através da derivação da equação de Landauer Büttiker! Procurando soluções para $\boldsymbol{g}^A_{L,L}$, $\boldsymbol{g}^R_{R,R}$ e $\boldsymbol{g}^A_{R,R}$ em termos de estados propagantes impondo condições de fronteira no infinito, é possível demonstrar as restantes equivalências.

5 Descrição de transporte em termos de Funções de Green

Imaginemos que temos um sistema em que para $t < 0$, os contactos estão desligados da região central. Os contactos estão a potenciais químicos distintos. A $t = 0$, ligamos os contactos e queremos calcular os contactos para $t \gg 0$.

Queremos então calcular a resposta do sistema (corrente) devido a uma perturbação (ligar os contactos). Mas ligar contactos é um efeito forte: temos de ir além de teoria de perturbações.

Vamos assumir que temos um sistema em equilíbrio termodinâmico. Para o sistema tripartido temos:

$$\rho(0) = \rho_L \otimes \rho_C \otimes \rho_R$$

$$H(0) = \begin{bmatrix} \boldsymbol{H}_R & 0 & 0 \\ 0 & \boldsymbol{H}_C & 0 \\ 0 & 0 & \boldsymbol{H}_L \end{bmatrix}$$

para $t > 0$:

$$H = \begin{bmatrix} \boldsymbol{H}_R & \boldsymbol{V}_{R,C} & 0 \\ \boldsymbol{V}_{C,R} & \boldsymbol{H}_C & \boldsymbol{V}_{C,L} \\ 0 & \boldsymbol{V}_{L,C} & \boldsymbol{H}_L \end{bmatrix}$$

e

$$\rho(t) = U(t,0)\rho(0)U(0,t)$$

onde

$$i\hbar\frac{\partial}{\partial t}U(t,0) = HU(t,0)$$

e

$$U(0,t) = U^{-1}(t,0) = U^{\dagger}(t,0)$$

Queremos calcular o valor médio de $I = I_{n+1\to n+1}$:

$$\begin{aligned} \langle I \rangle (t) &= \mathrm{Tr}\left[\rho(t)I\right] \\ &= \mathrm{Tr}\left[U(t,0)\rho(0)U(0,t)I\right] \\ &= \mathrm{Tr}\left[\rho(0)U(0,t)IU(t,0)\right] \end{aligned}$$

O operador corrente é dado por

$$\begin{aligned} I_{C\to R} &= \frac{dN_R}{dt} \\ &= \frac{i}{\hbar}\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & \boldsymbol{V}_{C,R} \\ 0 & -\boldsymbol{V}_{R,C} & 0 \end{bmatrix}. \end{aligned}$$

5.1 Representação de interação:

Tratar ligação de contactos como perturbação: $H = H_0 + V$. Onde

$$H_0 = \begin{bmatrix} \boldsymbol{H}_R & 0 & 0 \\ 0 & \boldsymbol{H}_C & 0 \\ 0 & 0 & \boldsymbol{H}_L \end{bmatrix}$$
$$V = \begin{bmatrix} 0 & \boldsymbol{V}_{R,C} & 0 \\ \boldsymbol{V}_{C,R} & 0 & \boldsymbol{V}_{C,L} \\ 0 & \boldsymbol{V}_{L,C} & 0 \end{bmatrix}$$

A representação de interação é definida como:

$$U(t,t') = e^{-iH_0(t-t_0)/\hbar}S(t,t')e^{iH_0\left(t'-t_0\right)/\hbar}$$
$$S(t,t') = e^{iH_0(t-t_0)/\hbar}U(t,t')e^{iH_0\left(t'-t_0\right)/\hbar}$$

Equação de movimento para $S(t,t')$:

$$i\hbar\frac{\partial}{\partial t}S(t,t') = V_I(t)S(t,t')$$

onde

$$V_I(t) = e^{iH_0 t/\hbar}Ve^{-iH_0 t/\hbar}.$$

E

$$-i\hbar\frac{\partial}{\partial t'}S(t,t') = S(t,t')V_I(t').$$

Formalmente, para $t > t'$

$$\begin{aligned}
S(t,t') &= 1 - \frac{i}{\hbar}\int_{t'}^{t} dt_1 V_I(t_1)S(t_1,t') \\
&= \sum_{n=0}^{+\infty}\left(-\frac{i}{\hbar}\right)^n \int_{t'}^{t} dt_1 \int_{t'}^{t_1} dt_2 ... \int_{t'}^{t_{n-1}} dt_n V_I(t_1)V_I(t_2)...V_I(t_n) \\
&= T\exp\left[-\frac{i}{\hbar}\int_{t'}^{t} dt_1 V_I(t_1)\right].
\end{aligned}$$

Para $t < t'$, temos

$$\begin{aligned}
S(t,t') &= 1 + \frac{i}{\hbar}\int_{t}^{t'} dt_1 S(t,t_1)V_I(t_1) \\
&= \sum_{n=0}^{+\infty}\left(\frac{i}{\hbar}\right)^n \int_{t}^{t'} dt_1 \int_{t}^{t_1} dt_2 ... \int_{t}^{t_{n-1}} dt_n V_I(t_n)...V_I(t_2)V_I(t_1) \\
&= \bar{T}\exp\left[\frac{i}{\hbar}\int_{t}^{t'} dt_1 V_I(t_1)\right].
\end{aligned}$$

é a perturbação na representação de interação. Nesta representação obtemos

$$\begin{aligned}
\langle I\rangle(t) &= \mathrm{Tr}\left[\rho(0)S(0,t)e^{iH_0 t/\hbar}Ie^{-iH_0 t/\hbar}S(t,0)\right] \\
&= \mathrm{Tr}\left[\rho(0)S(0,t)I_I(t)S(t,0)\right] \\
&= \sum_{n,m=0}^{+\infty}\left(\frac{i}{\hbar}\right)^n\left(-\frac{i}{\hbar}\right)^m \int_0^t dt_1 \int_0^{t_1} dt_2 ... \int_0^t dt'_1 \int_0^{t'_1} dt'_2 ... \times \\
&\qquad \langle ...V_I(t_2)V_I(t_1)I_I(t)V_I(t'_1)V_I(t'_2)...\rangle_0
\end{aligned}$$

5.2 Teorema de Wick/Gaudin

Como calcular os valores médios $\langle ...V_I(t_2)V_I(t_1)I_I(t)V_I(t'_1)V_I(t'_2)...\rangle_0$: teorema de Wick (ou Gaudin). Para um sistema de partículas livres em equilíbrio termodinâmico, valor médio de productos de operadores de criação/destruição é dado por todas as combinações possíveis (partículas indistinguíveis) de productos de valores médios de par criação-destruição (partículas livres). O sinal de cada termo é obtido dado pelo sinal da permutação de operadores (estatística das partículas) . Exemplo:

$$\left\langle c_1 c_2^\dagger c_3^\dagger c_4\right\rangle = \left\langle c_1 c_2^\dagger\right\rangle\left\langle c_3^\dagger c_4\right\rangle - \left\langle c_1 c_3^\dagger\right\rangle\left\langle c_2^\dagger c_4\right\rangle$$

Podemos então ordenar todos os operadores e depois aplicar o teorema de Gaudin. Vamos gerar:
(i) valores médios de operadores ordenados no tempo:

$$G^T_{\alpha\beta}(t,t') = -\frac{i}{\hbar}\left\langle Tc_\alpha(t)c_\beta^\dagger(t')\right\rangle;$$

(ii) valores médios de operadores anti-ordenados no tempo:

$$G^{\bar{T}}_{\alpha\beta}(t,t') = -\frac{i}{\hbar}\left\langle \bar{T}c_\alpha(t)c_\beta^\dagger(t')\right\rangle;$$

(iii) valor médios de operadores com ordem fixa:

$$G^{>}_{\alpha\beta}(t,t') = -\frac{i}{\hbar}\left\langle c_\alpha(t)c^\dagger_\beta(t')\right\rangle,$$
$$G^{<}_{\alpha\beta}(t,t') = \frac{i}{\hbar}\left\langle c^\dagger_\beta(t')c_\alpha(t)\right\rangle.$$

Temos um problema de contabilidade.

5.3 Formalismo de Keldysh

5.3.1 Contorno de Schwinger-Keldysh

Considerar um único contorno, o contorno de Schwinger-Keldysh

$$C = [t_0, t_\infty] \cup [t_\infty, t_0].$$

De tal forma que

$$\langle I\rangle(t) = \mathrm{Tr}\left[\rho(0)S_C I_I(t)\right]$$
$$S_C = T_C \exp\left[-\frac{i}{\hbar}\int_C ds_1 V_I(s_1)\right].$$

T_C é um operador de ordenação ao longo do contorno e

$$\int_C ds_1 ... = \int_{t_0}^{t_\infty} dt_+ - \int_{t_0}^{t_\infty} dt_-$$

E definimos uma função de Green ordenada no contorno

$$G^C_{\alpha\beta}(s,s') = -i\left\langle T_C c_\alpha(s)c^\dagger_\beta(s')\right\rangle.$$

(i) se $s = t_+$ e $s' = t'_+$: $G^C_{\alpha\beta}(t_+,t'_+) = G^T_{\alpha\beta}(t,t')$
(ii) se $s = t_-$ e $s' = t'_-$: $G^C_{\alpha\beta}(t_-,t'_-) = G^{\bar{T}}_{\alpha\beta}(t,t')$
(iii) se $s = t_+$ e $s' = t'_-$: $G^C_{\alpha\beta}(t_+,t'_-) = G^{<}_{\alpha\beta}(t,t')$
(iv) se $s = t_-$ e $s' = t'_+$: $G^C_{\alpha\beta}(t_-,t'_+) = G^{>}_{\alpha\beta}(t,t')$

5.3.2 Série de Dyson no contorno

Indo para uma representação de interação, obtemos

$$\begin{aligned} G^C_{\alpha\beta}(s,s') &= -\frac{i}{\hbar}\left\langle T_C \hat{c}_\alpha(s)\hat{c}^\dagger_\beta(s')\right\rangle \\ &= -\frac{i}{\hbar}\left\langle T_C e^{-\frac{i}{\hbar}\int_C ds_1 V_I(s_1)} c_\alpha(s)c^\dagger_\beta(s')\right\rangle_0 \\ &= -\frac{i}{\hbar}\frac{\left\langle T_C e^{-\frac{i}{\hbar}\int_C ds_1 V_I(s_1)} c_\alpha(s)c^\dagger_\beta(s')\right\rangle_0}{\left\langle T_C e^{-\frac{i}{\hbar}\int_C ds_1 V_I(s_1)}\right\rangle_0}. \end{aligned}$$

Se a perturbação V é um potencial de uma partícula, expandido em série de potências em $V_I(s_1)$, obtemos a série de Dyson:

$$\boldsymbol{G}^C(s,s') = \boldsymbol{g}^C(s,s') + \int_C ds_1 \boldsymbol{g}^C(s,s_1)V_I(s_1)\boldsymbol{G}^C(s_1,s').$$

Escrevendo:

$$\underline{\boldsymbol{G}}(t,t') = \begin{bmatrix} \boldsymbol{G}^T(t,t') & \boldsymbol{G}^<(t,t') \\ \boldsymbol{G}^>(t,t') & \boldsymbol{G}^{\bar{T}}(t,t') \end{bmatrix}$$

A equação de Dyson toma a forma

$$\begin{aligned} \begin{bmatrix} \boldsymbol{G}^T(t,t') & \boldsymbol{G}^<(t,t') \\ \boldsymbol{G}^>(t,t') & \boldsymbol{G}^{\bar{T}}(t,t') \end{bmatrix} &= \begin{bmatrix} \boldsymbol{g}^T(t,t') & \boldsymbol{g}^<(t,t') \\ \boldsymbol{g}^>(t,t') & \boldsymbol{g}^{\bar{T}}(t,t') \end{bmatrix} + \\ &+ \int_{t_0}^{+\infty} dt_1 \begin{bmatrix} \boldsymbol{g}^T(t,t_1) & \boldsymbol{g}^<(t,t_1) \\ \boldsymbol{g}^>(t,t_1) & \boldsymbol{g}^{\bar{T}}(t,t_1) \end{bmatrix} \begin{bmatrix} \boldsymbol{V}(t_1) & 0 \\ 0 & -\boldsymbol{V}(t_1) \end{bmatrix} \begin{bmatrix} \boldsymbol{G}^T(t_1,t') & \boldsymbol{G}^<(t_1,t') \\ \boldsymbol{G}^>(t_1,t') & \boldsymbol{G}^{\bar{T}}(t_1,t') \end{bmatrix} \end{aligned}$$

5.3.3 Regras de Langreth

As funções de Green não são todas independentes. Na realidade, pelas definições:

$$G^{T}_{\alpha\beta}(t,t') + G^{\bar{T}}_{\alpha\beta}(t,t') = G^{>}_{\alpha\beta}(t,t') + G^{<}_{\alpha\beta}(t,t')$$

Comos livres de considerar diferentes combinações de funções de Green. É usual definir:
(i) Função de Green Retardada:

$$G^{R}_{\alpha\beta}(t,t') = G^{T}_{\alpha\beta}(t,t') - G^{<}_{\alpha\beta}(t,t') = G^{>}_{\alpha\beta}(t,t') - G^{\bar{T}}_{\alpha\beta}(t,t') = -\frac{i}{\hbar}\Theta(t-t')\left\langle\left\{c_\alpha(t), c^\dagger_\beta(t')\right\}\right\rangle$$

(ii) Função de Green Avançada:

$$G^{A}_{\alpha\beta}(t,t') = G^{<}_{\alpha\beta}(t,t') - G^{\bar{T}}_{\alpha\beta}(t,t') = G^{T}_{\alpha\beta}(t,t') - G^{>}_{\alpha\beta}(t,t') = \frac{i}{\hbar}\Theta(-t't)\left\langle\left\{c_\alpha(t), c^\dagger_\beta(t')\right\}\right\rangle$$

Diferentes combinações lineares podem ser aplicadas através de multiplações por matrizes:

$$\begin{bmatrix} \boldsymbol{G}^{T}(t,t') & \boldsymbol{G}^{<}(t,t') \\ \boldsymbol{G}^{>}(t,t') & \boldsymbol{G}^{\bar{T}}(t,t') \end{bmatrix} \to \underline{M}^{-1} \begin{bmatrix} \boldsymbol{G}^{T}(t,t') & \boldsymbol{G}^{<}(t,t') \\ \boldsymbol{G}^{>}(t,t') & \boldsymbol{G}^{\bar{T}}(t,t') \end{bmatrix} \underline{N}^{-1}.$$

De forma que a equação de de Dyson pode ser escrita como

$$\begin{aligned} \underline{G} &= \underline{g} + \underline{g}\cdot\underline{V}\cdot\underline{G} \\ \underline{M}^{-1}\cdot\underline{G}\cdot\underline{N}^{-1} &= \underline{M}^{-1}\cdot\underline{g}\cdot\underline{N}^{-1} + \underline{M}^{-1}\cdot\underline{g}\cdot\underline{N}^{-1}\cdot\underline{N}\cdot\underline{V}\cdot\underline{M}\cdot\underline{M}^{-1}\cdot\underline{G}\cdot\underline{N}^{-1} \end{aligned}$$

Para

$$\begin{aligned} \underline{M} &= \begin{bmatrix} 1 & 0 \\ 1 & -1 \end{bmatrix}, \underline{M}^{-1} = \begin{bmatrix} 1 & 0 \\ 1 & -1 \end{bmatrix} \\ \underline{N} &= \begin{bmatrix} 1 & 0 \\ 1 & 1 \end{bmatrix}, \underline{N}^{-1} = \begin{bmatrix} 1 & 0 \\ -1 & 1 \end{bmatrix} \end{aligned}$$

Obtemos

$$\begin{aligned} \underline{M}^{-1}\cdot\underline{G}\cdot\underline{N}^{-1} &= \begin{bmatrix} 1 & 0 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} G^{T} & G^{<} \\ G^{>} & G^{\bar{T}} \end{bmatrix} \begin{bmatrix} 1 & 0 \\ -1 & 1 \end{bmatrix} \\ &= \begin{bmatrix} G^{T} & G^{<} \\ G^{T}-G^{>} & G^{<}-G^{\bar{T}} \end{bmatrix} \begin{bmatrix} 1 & 0 \\ -1 & 1 \end{bmatrix} \\ &= \begin{bmatrix} G^{T}-G^{<} & G^{<} \\ G^{T}-G^{>}-G^{<}+G^{\bar{T}} & G^{<}-G^{\bar{T}} \end{bmatrix} \\ &= \begin{bmatrix} G^{R} & G^{<} \\ 0 & G^{A} \end{bmatrix}. \end{aligned}$$

Também notamos que

$$\begin{aligned} \underline{N}\cdot\underline{V}\cdot\underline{M} &= \begin{bmatrix} 1 & 0 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} V & 0 \\ 0 & -V \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 1 & -1 \end{bmatrix} \\ &= \begin{bmatrix} V & 0 \\ V & -V \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 1 & -1 \end{bmatrix} \\ &= \begin{bmatrix} V & 0 \\ 0 & V \end{bmatrix}. \end{aligned}$$

Logo obtemos a seguinte equação:

$$\begin{aligned} \begin{bmatrix} \boldsymbol{G}^{R}(t,t') & \boldsymbol{G}^{<}(t,t') \\ 0 & \boldsymbol{G}^{A}(t,t') \end{bmatrix} &= \begin{bmatrix} \boldsymbol{g}^{R}(t,t') & \boldsymbol{g}^{<}(t,t') \\ 0 & \boldsymbol{g}^{A}(t,t') \end{bmatrix} + \\ &+ \int_{t_0}^{+\infty} dt_1 \begin{bmatrix} \boldsymbol{g}^{R}(t,t_1) & \boldsymbol{g}^{<}(t,t_1) \\ 0 & \boldsymbol{g}^{A}(t,t_1) \end{bmatrix} \begin{bmatrix} \boldsymbol{V}(t_1) & 0 \\ 0 & \boldsymbol{V}(t_1) \end{bmatrix} \begin{bmatrix} \boldsymbol{G}^{R}(t_1,t') & \boldsymbol{G}^{<}(t_1,t') \\ 0 & \boldsymbol{G}^{A}(t_1,t') \end{bmatrix} \end{aligned}$$

Notando que:

$$\left[\begin{array}{cc} g^R & g^< \\ 0 & g^A \end{array}\right]\left[\begin{array}{cc} V & 0 \\ 0 & V \end{array}\right]\left[\begin{array}{cc} G^R & G^< \\ 0 & G^A \end{array}\right] =$$

$$= \left[\begin{array}{cc} g^R & g^< \\ 0 & g^A \end{array}\right]\left[\begin{array}{cc} VG^R & VG^< \\ 0 & VG^A \end{array}\right]$$

$$= \left[\begin{array}{cc} g^R VG^R & g^R VG^< + g^< VG^A \\ 0 & g^A VG^A \end{array}\right].$$

Assim obtemos:

$$\begin{aligned}
\boldsymbol{G}^R(t,t') &= \boldsymbol{g}^R(t,t') + \int_{t_0}^{+\infty} dt_1 \boldsymbol{g}^R(t,t_1)\boldsymbol{V}(t_1)\boldsymbol{G}^R(t_1,t') \\
\boldsymbol{G}^A(t,t') &= \boldsymbol{g}^A(t,t') + \int_{t_0}^{+\infty} dt_1 \boldsymbol{g}^A(t,t_1)\boldsymbol{V}(t_1)\boldsymbol{G}^A(t_1,t') \\
\boldsymbol{G}^<(t,t') &= \boldsymbol{g}^<(t,t') + \int_{t_0}^{+\infty} dt_1 \boldsymbol{g}^R(t,t_1)\boldsymbol{V}(t_1)\boldsymbol{G}^<(t_1,t') \\
&+ \int_{t_0}^{+\infty} dt_1 \boldsymbol{g}^<(t,t_1)\boldsymbol{V}(t_1)\boldsymbol{G}^A(t_1,t').
\end{aligned}$$

Outras representações são possíveis. Por exemplo, escolhendo:

$$\begin{aligned}
\underline{M} &= \left[\begin{array}{cc} 1 & 1 \\ 0 & 1 \end{array}\right], \underline{M}^{-1} = \left[\begin{array}{cc} 1 & -1 \\ 0 & 1 \end{array}\right] \\
\underline{N} &= \left[\begin{array}{cc} 1 & 1 \\ 0 & -1 \end{array}\right], \underline{N}^{-1} = \left[\begin{array}{cc} 1 & 1 \\ 0 & -1 \end{array}\right]
\end{aligned}$$

Obtemos:

$$\left[\begin{array}{cc} \boldsymbol{G}^R(t,t') & 0 \\ \boldsymbol{G}^>(t,t') & \boldsymbol{G}^A(t,t') \end{array}\right] = \left[\begin{array}{cc} \boldsymbol{g}^R(t,t') & 0 \\ \boldsymbol{g}^>(t,t') & \boldsymbol{g}^A(t,t') \end{array}\right] +$$

$$+ \int_{t_0}^{+\infty} dt_1 \left[\begin{array}{cc} \boldsymbol{g}^R(t,t_1) & 0 \\ \boldsymbol{g}^>(t,t_1) & \boldsymbol{g}^A(t,t_1) \end{array}\right]\left[\begin{array}{cc} \boldsymbol{V}(t_1) & 0 \\ 0 & \boldsymbol{V}(t_1) \end{array}\right]\left[\begin{array}{cc} \boldsymbol{G}^R(t_1,t') & 0 \\ \boldsymbol{G}^>(t_1,t') & \boldsymbol{G}^A(t_1,t') \end{array}\right].$$

De onde obtemos, mais uma equação:

$$\begin{aligned}
\boldsymbol{G}^>(t,t') &= \boldsymbol{g}^>(t,t') + \int_{t_0}^{+\infty} dt_1 \boldsymbol{g}^R(t,t_1)\boldsymbol{V}(t_1)\boldsymbol{G}^>(t_1,t') \\
&+ \int_{t_0}^{+\infty} dt_1 \boldsymbol{g}^>(t,t_1)\boldsymbol{V}(t_1)\boldsymbol{G}^A(t_1,t').
\end{aligned}$$

5.4 Cálculo da corrente com o formalismo de Keldysh

Escrevendo o Hamiltoniano em segunda quantificação, temos

$$H = \left[\begin{array}{ccc} \boldsymbol{c}_R^\dagger & \boldsymbol{c}_C^\dagger & \boldsymbol{c}_L^\dagger \end{array}\right]\left[\begin{array}{ccc} \boldsymbol{H}_R & \boldsymbol{V}_{R,C} & 0 \\ \boldsymbol{V}_{C,R} & \boldsymbol{H}_C & \boldsymbol{V}_{C,L} \\ 0 & \boldsymbol{V}_{L,C} & \boldsymbol{H}_L \end{array}\right]\left[\begin{array}{c} \boldsymbol{c}_R \\ \boldsymbol{c}_C \\ \boldsymbol{c}_R \end{array}\right]$$

e o operador de corrente é

$$\begin{aligned}
I_{C\to R} &= \frac{dN_R}{dt} \\
&= \frac{i}{\hbar}\left[\begin{array}{ccc} \boldsymbol{c}_R^\dagger & \boldsymbol{c}_C^\dagger & \boldsymbol{c}_L^\dagger \end{array}\right]\left[\begin{array}{ccc} 0 & 0 & 0 \\ 0 & 0 & \boldsymbol{V}_{C,R} \\ 0 & -\boldsymbol{V}_{R,C} & 0 \end{array}\right]\left[\begin{array}{c} \boldsymbol{c}_R \\ \boldsymbol{c}_C \\ \boldsymbol{c}_R \end{array}\right] \\
&= \frac{i}{\hbar}\left(\boldsymbol{c}_C^\dagger \cdot \boldsymbol{V}_{C,R} \cdot \boldsymbol{c}_R - \boldsymbol{c}_R \cdot \boldsymbol{V}_{R,C} \cdot \boldsymbol{c}_C\right).
\end{aligned}$$

Temos então

$$\begin{aligned}\langle I_{C\to R}\rangle(t) &= \frac{i}{\hbar}\left(\left\langle \boldsymbol{c}_C^\dagger(t)\cdot\boldsymbol{V}_{C,R}\cdot\boldsymbol{c}_R(t)\right\rangle - \left\langle \boldsymbol{c}_R^\dagger(t)\cdot\boldsymbol{V}_{R,C}\cdot\boldsymbol{c}_C(t)\right\rangle\right)\\ &= \mathrm{Tr}\left[\boldsymbol{V}_{C,R}\cdot\boldsymbol{G}^<_{R,C}(t,t)\right] - \mathrm{Tr}\left[\boldsymbol{V}_{R,C}\cdot\boldsymbol{G}^<_{C,R}(t,t)\right]\end{aligned}$$

Vamos usar a equação de Dyson:

$$\begin{aligned}\begin{bmatrix}\underline{\boldsymbol{G}}_{L,L} & \underline{\boldsymbol{G}}_{L,C} & \underline{\boldsymbol{G}}_{L,R}\\ \underline{\boldsymbol{G}}_{C,L} & \underline{\boldsymbol{G}}_{C,C} & \underline{\boldsymbol{G}}_{C,R}\\ \underline{\boldsymbol{G}}_{R,L} & \underline{\boldsymbol{G}}_{R,C} & \underline{\boldsymbol{G}}_{R,R}\end{bmatrix} &= \begin{bmatrix}\underline{\boldsymbol{g}}_{L,L} & & \\ & \underline{\boldsymbol{g}}_{C,C} & \\ & & \underline{\boldsymbol{g}}_{R,R}\end{bmatrix} + \begin{bmatrix}\underline{\boldsymbol{g}}_{L,L} & & \\ & \underline{\boldsymbol{g}}_{C,C} & \\ & & \underline{\boldsymbol{g}}_{R,R}\end{bmatrix}\begin{bmatrix}0 & \underline{\boldsymbol{V}}_{R,C} & 0\\ \underline{\boldsymbol{V}}_{C,R} & 0 & \underline{\boldsymbol{V}}_{C,L}\\ 0 & \underline{\boldsymbol{V}}_{L,C} & 0\end{bmatrix}\begin{bmatrix}\underline{\boldsymbol{G}}_{L,L} & \underline{\boldsymbol{G}}_{L,C} & \underline{\boldsymbol{G}}\\ \underline{\boldsymbol{G}}_{C,L} & \underline{\boldsymbol{G}}_{C,C} & \underline{\boldsymbol{G}}\\ \underline{\boldsymbol{G}}_{R,L} & \underline{\boldsymbol{G}}_{R,C} & \underline{\boldsymbol{G}}\end{bmatrix}\\ &= \begin{bmatrix}\underline{\boldsymbol{g}}_{L,L} & & \\ & \underline{\boldsymbol{g}}_{C,C} & \\ & & \underline{\boldsymbol{g}}_{R,R}\end{bmatrix} + \begin{bmatrix}\underline{\boldsymbol{G}}_{L,L} & \underline{\boldsymbol{G}}_{L,C} & \underline{\boldsymbol{G}}_{L,R}\\ \underline{\boldsymbol{G}}_{C,L} & \underline{\boldsymbol{G}}_{C,C} & \underline{\boldsymbol{G}}_{C,R}\\ \underline{\boldsymbol{G}}_{R,L} & \underline{\boldsymbol{G}}_{R,C} & \underline{\boldsymbol{G}}_{R,R}\end{bmatrix}\begin{bmatrix}0 & \underline{\boldsymbol{V}}_{R,C} & 0\\ \underline{\boldsymbol{V}}_{C,R} & 0 & \underline{\boldsymbol{V}}_{C,L}\\ 0 & \underline{\boldsymbol{V}}_{L,C} & 0\end{bmatrix}\begin{bmatrix}\underline{\boldsymbol{g}}_{L,L} & & \\ & \underline{\boldsymbol{g}}_{C,C} & \\ & & \underline{\boldsymbol{g}}\end{bmatrix}\end{aligned}$$

De onde obtemos

$$\begin{aligned}\underline{\boldsymbol{G}}_{C,R} &= \underline{\boldsymbol{G}}_{C,C}\cdot\underline{\boldsymbol{V}}_{C,R}\cdot\underline{\boldsymbol{g}}_{R,R}\\ \underline{\boldsymbol{G}}_{R,C} &= \underline{\boldsymbol{g}}_{R,R}\cdot\underline{\boldsymbol{V}}_{R,C}\cdot\underline{\boldsymbol{G}}_{C,C}\end{aligned}$$

Obtemos também:

$$\underline{\boldsymbol{G}}_{C,C} = \underline{\boldsymbol{g}}_{C,C} + \underline{\boldsymbol{g}}_{C,C}\cdot\underline{\boldsymbol{V}}_{C,R}\cdot\underline{\boldsymbol{G}}_{R,C} + \underline{\boldsymbol{g}}_{C,C}\cdot\underline{\boldsymbol{V}}_{C,L}\cdot\underline{\boldsymbol{G}}_{L,C}$$

A equação para $\underline{\boldsymbol{G}}_{L,C}$ é dada por

$$\underline{\boldsymbol{G}}_{L,C} = \underline{\boldsymbol{g}}_{L,L}\cdot\underline{\boldsymbol{V}}_{L,C}\cdot\underline{\boldsymbol{G}}_{C,C}$$

Logo obtemos:

$$\underline{\boldsymbol{G}}_{C,C} = \underline{\boldsymbol{g}}_{C,C} + \underline{\boldsymbol{g}}_{C,C}\cdot\underline{\boldsymbol{V}}_{C,R}\cdot\underline{\boldsymbol{g}}_{R,R}\cdot\underline{\boldsymbol{V}}_{R,C}\cdot\underline{\boldsymbol{G}}_{C,C} + \underline{\boldsymbol{g}}_{C,C}\cdot\underline{\boldsymbol{V}}_{C,L}\cdot\underline{\boldsymbol{g}}_{L,L}\cdot\underline{\boldsymbol{V}}_{L,C}\cdot\underline{\boldsymbol{G}}_{C,C}.$$

Definindo

$$\begin{aligned}\underline{\boldsymbol{\Sigma}}_R &= \underline{\boldsymbol{V}}_{C,R}\cdot\underline{\boldsymbol{g}}_{R,R}\cdot\underline{\boldsymbol{V}}_{R,C}\\ \underline{\boldsymbol{\Sigma}}_L &= \underline{\boldsymbol{V}}_{C,L}\cdot\underline{\boldsymbol{g}}_{L,L}\cdot\underline{\boldsymbol{V}}_{L,C}\end{aligned}$$

temos

$$\underline{\boldsymbol{G}}_{C,C} = \underline{\boldsymbol{g}}_{C,C} + \underline{\boldsymbol{g}}_{C,C}\cdot\underline{\boldsymbol{\Sigma}}_R\cdot\underline{\boldsymbol{G}}_{C,C} + \underline{\boldsymbol{g}}_{C,C}\cdot\underline{\boldsymbol{\Sigma}}_L\cdot\underline{\boldsymbol{G}}_{C,C}$$

Usando as regras de Langreth, obtemos:

$$\begin{aligned}\boldsymbol{G}^<_{C,R} &= \boldsymbol{G}^R_{C,C}\cdot\boldsymbol{V}_{C,R}\cdot\boldsymbol{g}^<_{R,R} + \boldsymbol{G}^<_{C,C}\cdot\boldsymbol{V}_{C,R}\cdot\boldsymbol{g}^A_{R,R}\\ \boldsymbol{G}^>_{R,C} &= \boldsymbol{g}^R_{R,R}\cdot\boldsymbol{V}_{R,C}\cdot\boldsymbol{G}^<_{C,C} + \boldsymbol{g}^<_{R,R}\cdot\boldsymbol{V}_{R,C}\cdot\boldsymbol{G}^A_{C,C}\end{aligned}$$

e

$$\boldsymbol{G}^<_{C,C} = \boldsymbol{g}^<_{C,C} + \boldsymbol{g}^R_{C,C}\cdot\boldsymbol{\Sigma}^R\cdot\boldsymbol{G}^<_{C,C} + \boldsymbol{g}^R_{C,C}\cdot\boldsymbol{\Sigma}^<\cdot\boldsymbol{G}^A_{C,C} + \boldsymbol{g}^<_{C,C}\cdot\boldsymbol{\Sigma}^A\cdot\boldsymbol{G}^A_{C,C}.$$

Para a função retardada obtemos:

$$\boldsymbol{G}^R_{C,C} = \boldsymbol{g}^R_{C,C} + \boldsymbol{g}^R_{C,C}\cdot\boldsymbol{\Sigma}^R\cdot\boldsymbol{G}^R_{C,C}.$$

Escrevemos esta equação como:

$$\left[1 - \boldsymbol{g}^R_{C,C}\cdot\boldsymbol{\Sigma}^R\right]\boldsymbol{G}^<_{C,C} = \boldsymbol{g}^<_{C,C} + \boldsymbol{g}^R_{C,C}\cdot\boldsymbol{\Sigma}^<\cdot\boldsymbol{G}^A_{C,C} + \boldsymbol{g}^<_{C,C}\cdot\boldsymbol{\Sigma}^A\cdot\boldsymbol{G}^A_{C,C}.$$

Actuar com $\left[\boldsymbol{g}^R_{C,C}\right]^{-1} = i\hbar\partial_t - \boldsymbol{H}_C$ (notar que $[i\hbar\partial_t - \boldsymbol{H}_C]\,\boldsymbol{g}^<_{CC}(t,t') = 0$):

$$\left[\left[\boldsymbol{g}^R_{C,C}\right]^{-1} - \boldsymbol{\Sigma}^R\right]\boldsymbol{G}^<_{C,C} = \boldsymbol{\Sigma}^<\cdot\boldsymbol{G}^A_{C,C}$$

A solução é dada por

$$\boldsymbol{G}^<_{C,C}(t,t') = \boldsymbol{G}^R_{C,C}(t,0)\boldsymbol{g}^<_{C,C}(0,0)\boldsymbol{G}^A_{C,C}(0,t') + \boldsymbol{G}^R_{C,C}\cdot\boldsymbol{\Sigma}^<\cdot\boldsymbol{G}^A_{C,C}$$

Mais explicitamente, temos a equação de Keldysh:

$$\boldsymbol{G}^{<}_{C,C}(t,t') = \boldsymbol{g}^{<}_{C,C}(t,t') + \int dt_1 \int dt_2 \boldsymbol{G}^{R}_{C,C}(t,t_1) \cdot \boldsymbol{\Sigma}^{<}(t_1,t_2) \cdot \boldsymbol{G}^{A}_{C,C}(t_2,t')$$

O primeiro termo descreve a memória do sistema em relação ao estado inicial. Se os contactos são infinitos, para $t, t' \gg 0$, a memória é perdida e:

$$\boldsymbol{G}^{<}_{C,C}(t,t') \simeq \int dt_1 \int dt_2 \boldsymbol{G}^{R}_{C,C}(t,t_1) \cdot \boldsymbol{\Sigma}^{<}(t_1,t_2) \cdot \boldsymbol{G}^{A}_{C,C}(t_2,t')$$

Temos então:

$$\begin{aligned}
\langle I_{C\to R}\rangle(t) &= \mathrm{Tr}\left[\boldsymbol{V}_{C,R} \cdot \boldsymbol{G}^{<}_{R,C}(t,t)\right] - \mathrm{Tr}\left[\boldsymbol{V}_{R,C} \cdot \boldsymbol{G}^{<}_{C,R}(t,t)\right] \\
&= \mathrm{Tr}\left[\boldsymbol{V}_{C,R} \cdot \boldsymbol{g}^{R}_{R,R} \cdot \boldsymbol{V}_{R,C} \cdot \boldsymbol{G}^{<}_{C,C}\right](t,t) + \mathrm{Tr}\left[\boldsymbol{V}_{C,R} \cdot \boldsymbol{g}^{<}_{R,R} \cdot \boldsymbol{V}_{R,C} \cdot \boldsymbol{G}^{A}_{C,C}\right](t,t) \\
&- \mathrm{Tr}\left[\boldsymbol{V}_{R,C} \cdot \boldsymbol{G}^{R}_{C,C} \cdot \boldsymbol{V}_{C,R} \cdot \boldsymbol{g}^{<}_{R,R}\right](t,t) - \mathrm{Tr}\left[\boldsymbol{V}_{R,C} \cdot \boldsymbol{G}^{<}_{C,C} \cdot \boldsymbol{V}_{C,R} \cdot \boldsymbol{g}^{A}_{R,R}\right](t,t) \\
&= \int dt_1 \mathrm{Tr}\left[\boldsymbol{\Sigma}^{R}_{R}(t,t_1) \cdot \boldsymbol{G}^{<}_{C,C}(t_1,t) + \boldsymbol{\Sigma}^{<}_{R}(t,t_1) \cdot \boldsymbol{G}^{A}_{C,C}(t_1,t)\right] \\
&- \int dt_1 \mathrm{Tr}\left[\boldsymbol{G}^{R}_{C,C}(t,t_1) \cdot \boldsymbol{\Sigma}^{<}_{R}(t_1,t) + \boldsymbol{G}^{<}_{C,C}(t,t_1) \cdot \boldsymbol{\Sigma}^{A}_{R}(t_1,t)\right].
\end{aligned}$$

Aproximação de longos tempos. Para $t \gg 0$, ocorre perda de memória e as funções tornam-se invariantes de translação temporal:

$$G(t,t') \to G(t-t')$$

Tomando o limite $t \to \infty$, e fazendo uma transformada de Fourier obtemos:

$$\begin{aligned}
\langle I_{C\to R}\rangle &= \lim_{t\to\infty} \langle I_{C\to R}\rangle(t) \\
&= \frac{1}{\hbar}\int \frac{dE}{2\pi} \mathrm{Tr}\left[\boldsymbol{\Sigma}^{R}_{R}(E) \cdot \boldsymbol{G}^{<}_{C,C}(E) + \boldsymbol{\Sigma}^{<}_{R}(E) \cdot \boldsymbol{G}^{A}_{C,C}(E)\right] \\
&= -\frac{1}{\hbar}\int \frac{dE}{2\pi} \mathrm{Tr}\left[\boldsymbol{G}^{R}_{C,C}(E) \cdot \boldsymbol{\Sigma}^{<}_{R}(E) + \boldsymbol{G}^{<}_{C,C}(E) \cdot \boldsymbol{\Sigma}^{A}_{R}(E)\right] \\
&= \frac{1}{\hbar}\int \frac{dE}{2\pi} \mathrm{Tr}\left[\left(\boldsymbol{\Sigma}^{R}_{R}(E) - \boldsymbol{\Sigma}^{A}_{R}(E)\right) \cdot \boldsymbol{G}^{<}_{C,C}(E) + \boldsymbol{\Sigma}^{<}_{R}(E) \cdot \left(\boldsymbol{G}^{A}_{C,C}(E) - \boldsymbol{G}^{R}_{C,C}(E)\right)\right]
\end{aligned}$$

Agora usamos a equação de Keldysh obtendo

$$\begin{aligned}
\langle I_{C\to R}\rangle &= \frac{1}{\hbar}\int \frac{dE}{2\pi} \mathrm{Tr}\left[\left(\boldsymbol{\Sigma}^{R}_{R}(E) - \boldsymbol{\Sigma}^{A}_{R}(E)\right) \cdot \boldsymbol{G}^{R}_{C,C}(E) \cdot \boldsymbol{\Sigma}^{<}(E) \cdot \boldsymbol{G}^{A}_{C,C}(E)\right] \\
&+ \frac{1}{\hbar}\int \frac{dE}{2\pi} \mathrm{Tr}\left[\boldsymbol{\Sigma}^{<}_{R}(E) \cdot \left(\boldsymbol{G}^{A}_{C,C}(E) - \boldsymbol{G}^{R}_{C,C}(E)\right)\right].
\end{aligned}$$

Escrevemos agora

$$\begin{aligned}
\boldsymbol{\Gamma}_{R/L}(E) &= i\left(\boldsymbol{\Sigma}^{R}_{R/L}(E) - \boldsymbol{\Sigma}^{A}_{R/L}(E)\right), \\
\boldsymbol{\Sigma}^{<}_{R/L}(E) &= i f_{R/L}(E) \boldsymbol{\Gamma}_{L/R}(E).
\end{aligned}$$

Obtemos então

$$\begin{aligned}
\langle I_{C\to R}\rangle &= \frac{1}{\hbar}\int \frac{dE}{2\pi} \mathrm{Tr}\left[-i\boldsymbol{\Gamma}_{R}(E) \cdot \boldsymbol{G}^{R}_{C,C}(E) \cdot i\left(f_L(E)\boldsymbol{\Gamma}_L(E) + f_R(E)\boldsymbol{\Gamma}_R(E)\right) \cdot \boldsymbol{G}^{A}_{C,C}(E)\right] \\
&+ \frac{1}{\hbar}\int \frac{dE}{2\pi} \mathrm{Tr}\left[i f_R(E)\boldsymbol{\Gamma}_R(E) \cdot \left(\boldsymbol{G}^{A}_{C,C}(E) - \boldsymbol{G}^{R}_{C,C}(E)\right)\right] \\
&= \frac{1}{\hbar}\int \frac{dE}{2\pi} f_L(E) \mathrm{Tr}\left[\boldsymbol{\Gamma}_R(E) \cdot \boldsymbol{G}^{R}_{C,C}(E) \cdot \boldsymbol{\Gamma}_L(E) \cdot \boldsymbol{G}^{A}_{C,C}(E)\right] \\
&+ \frac{1}{\hbar}\int \frac{dE}{2\pi} f_R(E) \mathrm{Tr}\left[\boldsymbol{\Gamma}_R(E) \cdot i\left(\boldsymbol{G}^{A}_{C,C}(E) - \boldsymbol{G}^{R}_{C,C}(E)\right) + \boldsymbol{\Gamma}_R(E) \cdot \boldsymbol{G}^{R}_{C,C}(E) \cdot \boldsymbol{\Gamma}_R(E) \cdot \boldsymbol{G}^{A}_{C,C}(E)\right]
\end{aligned}$$

Definimos a função espectral como

$$
\begin{aligned}
\boldsymbol{A}_{CC}(E) &= i\left[\boldsymbol{G}^{R}_{C,C}(E) - \boldsymbol{G}^{A}_{C,C}(E)\right] \\
&= \boldsymbol{G}^{R}_{C,C}(E)\cdot\boldsymbol{\Gamma}(E)\cdot\boldsymbol{G}^{A}_{C,C}(E) \\
&= \boldsymbol{G}^{R}_{C,C}(E)\cdot(\boldsymbol{\Gamma}_L(E)+\boldsymbol{\Gamma}_R(E))\cdot\boldsymbol{G}^{A}_{C,C}(E).
\end{aligned}
$$

Obtemos então

$$
\begin{aligned}
\langle I_{C\to R}\rangle &= \frac{1}{\hbar}\int\frac{dE}{2\pi}f_L(E)\mathrm{Tr}\left[\boldsymbol{\Gamma}_R(E)\cdot\boldsymbol{G}^{R}_{C,C}(E)\cdot\boldsymbol{\Gamma}_L(E)\cdot\boldsymbol{G}^{A}_{C,C}(E)\right] \\
&+ \frac{1}{\hbar}\int\frac{dE}{2\pi}f_R(E)\mathrm{Tr}\left[-\boldsymbol{\Gamma}_L(E)\cdot\boldsymbol{G}^{R}_{C,C}(E)\cdot(\boldsymbol{\Gamma}_L(E)+\boldsymbol{\Gamma}_R(E))\cdot\boldsymbol{G}^{A}_{C,C}(E)+\boldsymbol{\Gamma}_R(E)\cdot\boldsymbol{G}^{R}_{C,C}(E)\cdot\boldsymbol{\Gamma}_R(E)\cdot\boldsymbol{G}^{A}_{C,C}(E)\right] \\
&= \frac{1}{\hbar}\int\frac{dE}{2\pi}f_L(E)\mathrm{Tr}\left[\boldsymbol{\Gamma}_R(E)\cdot\boldsymbol{G}^{R}_{C,C}(E)\cdot\boldsymbol{\Gamma}_L(E)\cdot\boldsymbol{G}^{A}_{C,C}(E)\right] \\
&+ \frac{1}{\hbar}\int\frac{dE}{2\pi}f_R(E)\mathrm{Tr}\left[-\boldsymbol{\Gamma}_R(E)\cdot\boldsymbol{G}^{R}_{C,C}(E)\cdot\boldsymbol{\Gamma}_L(E)\cdot\boldsymbol{G}^{A}_{C,C}(E)-\boldsymbol{\Gamma}_R(E)\cdot\boldsymbol{G}^{R}_{C,C}(E)\cdot\boldsymbol{\Gamma}_R(E)\cdot\boldsymbol{G}^{A}_{C,C}(E)+\boldsymbol{\Gamma}_R(E)\cdot\boldsymbol{G}^{R}_{C,C}(E)\cdot\right. \\
&= \frac{1}{\hbar}\int\frac{dE}{2\pi}\left[f_L(E)-f_R(E)\right]\mathrm{Tr}\left[\boldsymbol{\Gamma}_R(E)\cdot\boldsymbol{G}^{R}_{C,C}(E)\cdot\boldsymbol{\Gamma}_L(E)\cdot\boldsymbol{G}^{A}_{C,C}(E)\right]
\end{aligned}
$$

A currente de carge é então dada por

$$
I^{e}_{L\to R} = -\frac{e}{\hbar}\int\frac{dE}{2\pi}\left[f_L(E)-f_R(E)\right]\mathrm{Tr}\left[\boldsymbol{\Gamma}_R(E)\cdot\boldsymbol{G}^{R}_{C,C}(E)\cdot\boldsymbol{\Gamma}_L(E)\cdot\boldsymbol{G}^{A}_{C,C}(E)\right].
$$