An Overview of the NEGF Formalism

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UG RnD, May 2024

NEGF formalism

Fundamental equations governing NEGF

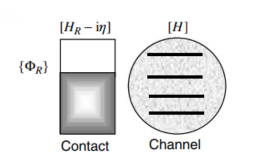


Figure: Channel contains no electrons and is disconnected from the contact where the electrons occupy the states described by $\{\Phi_R\}$

NEGF formalism

Fundamental equations governing NEGF

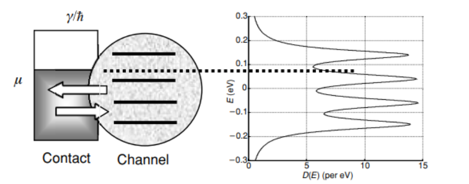
$$\begin{array}{ccc} & \text{contact} & \text{device} \\ \text{contact} & \multicolumn{2}{c}{\multirow{2}{*}{}} \\ \text{device} & & \end{array} \quad \begin{pmatrix} EI_R - H_R + i\eta & -\tau^\dagger \\ -\tau & EI - H \end{pmatrix} \begin{Bmatrix} \Phi_R + \chi \\ \psi \end{Bmatrix} = \begin{Bmatrix} S_R \\ 0 \end{Bmatrix}$$

$$G_R = [EI_R - H_R + i\eta]^{-1}$$
$$\{\chi\} = G_R \, \tau^\dagger \{\psi\}$$
$$\{\psi\} = G \, \{S\}$$

where

$$G = [EI - H - \Sigma]^{-1}$$
$$\Sigma = \tau G_R \tau^\dagger, \quad S = \tau \Phi_R$$

The contact/reservoir has a near-continuous distribution of energy levels, whereas the channel has a discrete set of energy levels. When the channel is coupled to a contact, one would expect an intermediate state of such energy levels- something in between a continuous distribution and discrete levels. This also implies that the energy levels within the channel are no longer eigenvalues of the Hamiltonian, $[H]$, but act as independent variables.



LDOS:

$$D(\vec{r};E) = \sum_{\alpha} |\Phi_{\alpha}(\vec{r})|^2 \, \delta(E-\epsilon_{\alpha}),$$

which is the diagonal element of the spectral matrix, $[A(E)]$:

$$A(\vec{r},\vec{r'};E) = 2\pi \sum_{\alpha} \phi_{\alpha}(\vec{r}) \, \delta(E-\epsilon_{\alpha}) \, \phi^{*}_{\alpha}(\vec{r'})$$

In matrix notation, $[A(E)] = 2\pi\delta(E[I]-[H])$, $D(E) = \frac{1}{2\pi}\mathrm{Tr}[A(E)]$

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Level broadening and LDOS

$$2\pi\delta(E-\epsilon_\alpha) = \left[\frac{2\eta}{(E-\epsilon_\alpha)^2+\eta^2}\right]_{\eta\to 0^+}$$

the spectral matrix can be expressed as:

$$[A(E)] = i[G(E) - G^\dagger(E)]$$

where

$$\text{Retarded Green's function}: G(E) = [(E+i0^+)I - H]^{-1}$$

$$\text{Advanced Green's function}: G^\dagger(E) = [(E-i0^+)^{-1}I - H]^{-1}$$

Note that the above expressions hold true for the reservoir/contact Green functions. The equivalent device/channel Green functions are given by:

$$\text{Retarded Green's function}: G(E) = [(E+i0^+)I - H - \tau G_R \tau^\dagger]^{-1}$$

$$\text{Advanced Green's function}: G^\dagger(E) = [(E-i0^+)^{-1}I - H - \tau G_R \tau^\dagger]^{-1}$$

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Green's functions in time domain

$[\tilde{G}^R(t)]$: Fourier transform of $[G^R(E)]$

$$[\tilde{G}^R(t)] = -\frac{i}{\hbar}\nu(t)e^{-i0^+t}\begin{bmatrix} e^{-i\epsilon_1 t/\hbar} & 0 & 0 & \dots \\ 0 & e^{-i\epsilon_2 t/\hbar} & 0 & \dots \\ 0 & 0 & e^{-i\epsilon_3 t/\hbar} & \dots \\ \dots & \dots & \dots & \dots \end{bmatrix}$$

Similarly,

$$[\tilde{G}^A(t)] = \frac{i}{\hbar}\nu(-t)e^{i0^+t}\begin{bmatrix} e^{-i\epsilon_1 t/\hbar} & 0 & 0 & \dots \\ 0 & e^{-i\epsilon_2 t/\hbar} & 0 & \dots \\ 0 & 0 & e^{-i\epsilon_3 t/\hbar} & \dots \\ \dots & \dots & \dots & \dots \end{bmatrix}$$

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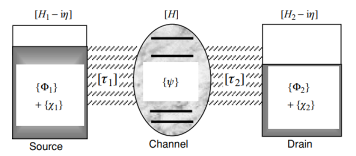
Channel connected to two contacts



$$\begin{pmatrix} EI - H_1 + i\eta & -\tau_1^\dagger & 0 \\ -\tau_1 & EI - H & -\tau_2 \\ 0 & -\tau_2^\dagger & EI - H_2 + i\eta \end{pmatrix} \begin{Bmatrix} \Phi_1 + \chi_1 \\ \psi \\ \Phi_2 + \chi_2 \end{Bmatrix} = \begin{Bmatrix} S_1 \\ 0 \\ S_2 \end{Bmatrix}$$

Channel Green's function, $G = [EI - H - \Sigma_1 - \Sigma_2]^{-1}$

Source term, $S = S_1 + S_2 = \tau_1\{\Phi_1\} + \tau_2\{\Phi_2\}$

Spectral function, $A = A_1 + A_2 = G(\Gamma_1 + \Gamma_2)G^\dagger$

NEGF formalism

Channel connected to two contacts

$$[\rho] = \int_{-\infty}^{+\infty} \frac{dE}{2\pi} \, [G^n(E)]$$

$$I_i = -\frac{q}{h} \int_{-\infty}^{+\infty} dE \, \{\underbrace{\mathrm{Tr}[\Gamma_i A] f_i}_{\text{Inflow}} - \underbrace{\mathrm{Tr}[\Gamma_i G^n]}_{\text{Outflow}}\}$$

$$\overline{T}(E) = \mathrm{Tr}[\Gamma_2 G \Gamma_1 G^\dagger]$$

where $[G^n] = [A_1] f_1 + [A_2] f_2 = G \Sigma_{in} G^\dagger = G\{[\Gamma_1] f_1 + [\Gamma_2] f_2\} G^\dagger$

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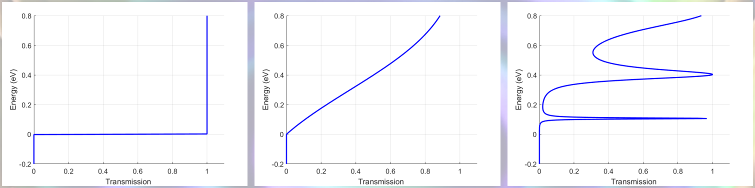
1-D examples



(a) Ballistic device (b) Tunneling device (c) RTD

Figure: Transmission function for different devices

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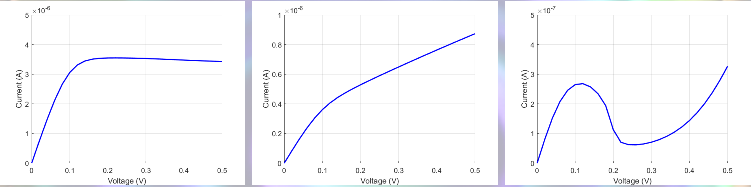
1-D examples



(a) Ballistic device (b) Tunneling device (c) RTD

Figure: I-V characteristics for different devices

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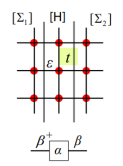
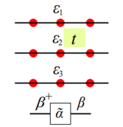
2-D conductors





where

$$\alpha = \begin{bmatrix} \epsilon & t & 0 \\ t & \epsilon & t \\ 0 & t & \epsilon \end{bmatrix}, \ \beta = \begin{bmatrix} t & 0 & 0 \\ 0 & t & 0 \\ 0 & 0 & t \end{bmatrix}$$

A basis transformation can be done such that α is diagonalized:

$$\tilde{\alpha} = V^{\dagger}\alpha V, \quad \tilde{\beta} = \beta$$

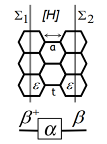
In the transformed basis, the 2D conductors can be visualized as a set of independent 1D conductors, with diagonal elements $\epsilon_n = \epsilon - 2t\ cos(k_n a)$, where $k_n a = \frac{n\pi}{N+1}$.

Previously shown transformations convert the lattice basis to an abstract mode basis.

$$\underbrace{\tilde{X}}_{\text{Mode basis}} = V^{\dagger} \underbrace{X}_{\text{Lattice basis}} V$$

$$\underbrace{X}_{\text{Lattice basis}} = V \underbrace{\tilde{X}}_{\text{Mode basis}} V^{\dagger}$$

$$\tilde{\Sigma}_1 = \begin{bmatrix} te^{ik_1 a} & 0 & 0 & \dots \\ 0 & te^{ik_2 a} & 0 & \dots \\ 0 & 0 & te^{ik_3 a} & \dots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix}$$



Recursive relation:

$$g_2^{-1} = (E + i0^+)I - \alpha - \beta^\dagger g_2 \beta$$

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Graphene