Introduction to Quantum transport

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Chapter 1

NEGF

Theory taken from QuantumATK paper, which is the clearest example I can find.

The NEGF key quantity to calculate is the retarded Green's function matrix for the central region. It is calculated from the central-region Hamiltonian matrix H and overlap matrix S by adding the electrode self-energies,

$$G(\varepsilon) = [(\varepsilon + i\delta_+)S - H - \Sigma^{L}(\varepsilon) - \Sigma^{R}(\varepsilon)]^{-1}, \qquad (1.1)$$

where δ_+ is an infinitesimal positive number. Calculation of G at a specific energy ε requires inversion of the central-region Hamiltonian matrix.

The electron density is given in terms of the electron density matrix. We split the density matrix into left and right contributions,

$$D = D^{L} + D^{R}, \qquad (1.2)$$

The left contribution is calculated using the NEGF method as

$$D^{L} = \int \rho^{L}(\varepsilon) f\left(\frac{\varepsilon - \mu_{L}}{k_B T_{L}}\right) d\varepsilon, \qquad (1.3)$$

where

$$\rho^{L}(\varepsilon) = \frac{1}{2\pi} G(\varepsilon) \Gamma^{L}(\varepsilon) G^{\dagger}(\varepsilon) \qquad (1.4)$$

is the spectral density matrix, expressed in terms of the retarded Green's function G

and the broadening function of the left electrode,

$$\Gamma^{\mathrm{L}} = \frac{1}{\mathbf{i}}\left(\Sigma^{\mathrm{L}} - (\Sigma^{\mathrm{L}})^{\dagger}\right) \tag{1.5}$$

which is given by the left electrode self-energy Σ^{L}. Note that while there is a non-equilibrium electron distribution in the central region, the electron distribution in the left electrode is described by a Fermi–Dirac distribution f with an electron temperature T_{L}.

The integral in 1.3 requires a dense set of energy points due to the rapid variation of the spectral density along the real axis. We therefore divide the integral into an equilibrium part, which can be integrated on a complex contour, and a non-equilibrium part, which needs to be integrated along the real axis, but only for energies within the bias window.

We have

$$D = D_{\mathrm{eq}}^{\mathrm{L}} + \Delta_{\mathrm{neq}}^{\mathrm{R}} \tag{1.6}$$

where

$$D_{\mathrm{eq}}^{\mathrm{L}} = \int \mathrm{d}\varepsilon (\rho^{\mathrm{L}}(\varepsilon) + \rho^{\mathrm{R}}(\varepsilon) + \rho^{\mathrm{B}}(\varepsilon)) f\left(\frac{\varepsilon - \mu_{\mathrm{L}}}{k_B T_{\mathrm{L}}}\right) \mathrm{d}\varepsilon, \tag{1.7}$$

$$\Delta_{\mathrm{neq}}^{\mathrm{R}} = \int \mathrm{d}\varepsilon \rho^{\mathrm{R}}(\varepsilon) \left[f\left(\frac{\varepsilon - \mu_{\mathrm{R}}}{k_B T_{\mathrm{R}}}\right) - f\left(\frac{\varepsilon - \mu_{\mathrm{L}}}{k_B T_{\mathrm{L}}}\right) \right], \tag{1.8}$$

where ρ^{B} is the density of states of any bound states in the central region.

Equivalently, we could write the density matrix as

$$D = D_{\mathrm{eq}}^{\mathrm{R}} + \Delta_{\mathrm{neq}}^{\mathrm{L}} \tag{1.9}$$

where L and R are exchanged in (59) and (60). Due to the finite accuracy of the integration along the real axis, (58) and (61) are numerically different. We therefore use a double contour, where (58) and (61) are combined

$$D_{ij} = W_{ij}^{\mathrm{L}} \left[D_{ij,\mathrm{eq}}^{\mathrm{L}} + \Delta_{ij,\mathrm{neq}}^{\mathrm{R}} \right] + W_{ij}^{\mathrm{R}} \left[D_{ij,\mathrm{eq}}^{\mathrm{R}} + \Delta_{ij,\mathrm{neq}}^{\mathrm{L}} \right] \tag{1.10}$$

with weights W_{ij}^{L} and W_{ij}^{R} for each matrix element ij. QuantumATK calculates these weights from the non-equilibrium atom Mulliken populations, while in this work we adopt the TranSIESTA approach which uses directly the non-equilibrium density to weight each matrix element individually. As the matrix elements are complex, we use the square of the densities to calculate the weight as

$$W_{ij}^{\mathrm{L}} = \frac{(\Delta_{ij,\mathrm{neq}}^{\mathrm{L}})^2}{(\Delta_{ij,\mathrm{neq}}^{\mathrm{L}})^2 + (\Delta_{ij,\mathrm{neq}}^{\mathrm{R}})^2}. \tag{1.11}$$