ECE 659: Quantum Transport Spring 2009

EE 117, MWF 930A-1020P

Course website: ***http://cobweb.ecn.purdue.edu/%7Edatta/659.htm***

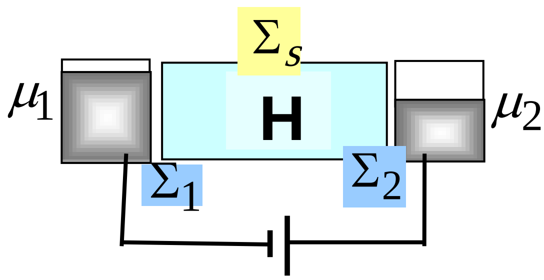
Lecture videos posted at https://nanohub.org/resources/6172/

"Input": H-matrix parameters chosen appropriately to match energy levels or dispersion relations. Σ_j ***for terminal 'j' is in general obtained from*** $\tau_j g_j \tau_j^+$ ***where the surface Green function 'g' is calculated from a recursive relation:*** $g^{-1} = EI - \alpha - \beta g \beta^+$.

$$\Gamma_j = i[\Sigma_j - \Sigma_j^+],\ \Gamma_S = i[\Sigma_S - \Sigma_S^+]$$

$$\Sigma \equiv \Sigma_s + \sum_j \Sigma_j,$$

and $$\Sigma^{in} \equiv \Sigma_s^{in} + \sum_j \Sigma_j^{in}$$



NEGF equations:

1. $G(E) = [EI - H - \Sigma_1 - \Sigma_2 - \Sigma_S]^{-1}$

2. $[G^n(E)] = [G\Sigma^{in}G^+]$

3. $A(E) = i[G - G^+] = G\Gamma G^+ = G^+\Gamma G$

4. $ih_{op} \mp [HG^n - G^n H] + [\Sigma G^n - G^n \Sigma^+] + [\Sigma^{in} G^+ - G\Sigma^{in}]$

4a. $I_{a\to b}(E) = \frac{q}{h} i[H_{ab}G^n_{ba} - G^n_{ab}H_{ba}]$ ***a, b: Internal Points***

4b. $I_i(E) = \frac{q}{h}((Trace[\Sigma_i^{in} A - \Gamma_i G^n])$ ***Current/energy at terminal 'i'***

4c. $I_i(E) = \frac{q}{h} \sum_j Trace[\Gamma_i G \Gamma_j G^+](f_i(E) - f_j(E))$

(***used only if*** Σ_s ***is zero: coherent transport*****)**

Note: $\Sigma_j^{in} = \Gamma_j f_j$ ***, but*** Σ_s^{in} ***cannot in general be written as*** $\Gamma_s f_s$.

Instead it has to be calculated self-consistently as summarized on next page.

A. For elastic scatterers in equilibrium:

$$[\Sigma_s] = D[G],\ [\Sigma_s^{in}] = D[G^n] \quad \textit{(S)}$$

where $D = U_s U_s^*$ describes incoherent processes (no relation to density of states D(E)).

B. For inelastic scatterers, with dissipation occurring due to interaction with a reservoir having a spectrum $D(+\varepsilon)$ for absorption and $D(-\varepsilon)$ for emission, See Section 10.3, page 271 of text (QTAT, Quantum Transport, Atom to Transistor):

Replace (S) with

$$[\Sigma_s^{in}(E)] = D(+\varepsilon)\,[G^n(E-\varepsilon)]$$

$$[\Gamma_s(E)] = D(+\varepsilon)\,[G^n(E-\varepsilon)] + D(+\varepsilon)\,[G^p(E+\varepsilon)]$$

(Note that $G^p(E)$ is the "hole density" given by $A(E) - G^n(E)$)

$$[\Sigma_s(E)] = \underbrace{[h(E)]}_{\substack{\text{Hilbert}\\ \text{Transform}}} - \frac{i}{2}[\Gamma_s(E)]$$

For a brief discussion of Hilbert transform see QTAT, top of page 206.

More generally, replace (S) with (summation over repeated indices is implied)

(S1) $$\left[\Sigma_s^{in}(E)\right]_{ij} = D_{ik;jl}(+\varepsilon)\left[G^n(E-\varepsilon)\right]_{kl}$$

(S2) $$\left[\Gamma_s(E)\right]_{ij} = D_{ik;jl}(+\varepsilon)\left[G^n(E-\varepsilon)\right]_{kl} + D_{lj;ki}(+\varepsilon)\left[G^p(E+\varepsilon)\right]_{kl}$$

(S3) $$[\Sigma_s(E)]_{ij} = \underbrace{[h(E)]_{ij}}_{\substack{\text{Hilbert}\\ \text{Transform}}} - \frac{i}{2}[\Gamma_s(E)]_{ij}$$

$$D_{ik;jl} = [U_s]_{ik}\,[U_s]_{jl}^*$$

If scatterers are in equilibrium with temperature T, then $\dfrac{D_{ik;jl}(+\varepsilon)}{D_{lj;ki}(-\varepsilon)} = e^{-\varepsilon/k_B T}$

Can show using (S1) and (S2) that the integrated scattering current is zero, though it may not be zero at each energy E: $\int dE\ I_i(E) = \dfrac{q}{h}\int dE\ Trace[\Sigma_s^{in} A - \Gamma_s G^n]$ ***= 0***