ECE 659: Quantum Transport Spring 2009

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

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

Fermi function: $f(E) = 1/(1+\exp((E-\mu)/kT))$

Current $I = \dfrac{q}{h}\int dE\, \pi\gamma\, D(E)\,(f_1(E)-f_2(E))$

Ballistic / diffusive transport: $\gamma = \hbar v_z / L$, $I = q\int dE\, \underbrace{\dfrac{D v_z}{2L}}_{\equiv \tilde{M}(E)/h}\,(f^+(E)-f^-(E))$

$$= \quad q\int dE\, \frac{D(E)}{2L}\,\frac{v_z\lambda}{\lambda+L}\,(f_1(E)-f_2(E))\,, \quad \lambda = 2v_z\tau$$

Electron density: $n(z,E) \;=\; \dfrac{D(z,E)}{2L}\,(f^+(z,E)+f^-(z,E))$

$$\frac{df^+}{dz} = \frac{df^-}{dz} = -\frac{f^+-f^-}{\lambda}\,, \quad \lambda \equiv 2v_z\tau$$

$$f^+(z,E)-f^-(z,E) = \frac{\lambda}{\lambda+L}(f_1(E)-f_2(E))$$

Linear Response: $I \approx \displaystyle\int dE\left(-\frac{\partial f}{\partial E}\right)\tilde{I}(E)\,, \quad \Delta\mu << kT$

$$\tilde{I} \approx \quad q\,\frac{D(E)}{2L}v_z\,(\mu^+-\mu^-) = \quad q^2\;\frac{D(E)}{2L}\,\frac{v_z\lambda}{\lambda+L}\left(\frac{\mu_1-\mu_2}{q}\right)$$

$$= \quad \underbrace{q^2\;\frac{D(E)}{WL}\,\frac{v^2\tau}{d}}_{\equiv\tilde{\sigma}(E)}\,\frac{W}{\lambda+L}V$$ ***(d=2 for 2D, 3 for 3D)***

$\tilde{I} = \quad \tilde{\sigma}\,\dfrac{W}{\lambda+L}\;V \quad \rightarrow$, ***if contact resistance is eliminated*** $\tilde{I} = \tilde{\sigma}\,\dfrac{W}{L}\;V$

$$\sigma_{zz} = \quad \int dE\left(-\frac{\partial f}{\partial E}\right)\tilde{\sigma}(E)\,, \quad \sigma_{zx} \approx \quad \int dE\left(-\frac{\partial f}{\partial E}\right)\tilde{\sigma}(E)\,\omega_c\tau$$

where $\tilde{\sigma}(E) \equiv \quad q^2\,\dfrac{D(E)}{WL}\,\dfrac{v^2\tau}{d}$, cf. Eqs.(4.33) and (4.60) in

Lundstrom, Fundamentals of Carrier Transport, Cambridge (2000).

$$\{i^-\} = \quad [S]\{i^+\} = \quad \underbrace{[S][M]}_{\equiv[\bar{S}]}\{\mu^+\}$$

Two-probe conductance,

$$Y = \quad (q^2/h)\,[I-S]\,[M] = \quad (q^2/h)\,[M-\bar{S}] \qquad \textbf{\textit{(Total)}}$$

$$Y = \quad (q^2/h)\,2\,[I-S]\;[I+S]^{-1}\;[M] \;=\; (q^2/h)\,2\,[M-\bar{S}]\;[M+\bar{S}]^{-1}\,[M] \textbf{\textit{(Channel only)}}$$

Four-probe conductance, $S = \begin{bmatrix} A & C \\ D & B \end{bmatrix}$, $\qquad P = \quad [A]+[C]\,[I-B]^{-1}\,[D]$

$$\bar{A} \equiv \quad [A][M_A], \quad \bar{B} \equiv \quad [B][M_B], \quad \bar{C} \equiv \quad [C][M_B], \quad \bar{D} \equiv \quad [D][M_A]$$

$$[\bar{P}] \equiv [P][M_A] = [\bar{A}] + [\bar{C}]\,[M_B - \bar{B}]^{-1}\,[\bar{D}]$$

$$\rightarrow \quad Y_{2pt} = \frac{i_A}{V_A} = \quad (q^2/h)\,[I-P]\,[M_A] = \quad (q^2/h)\,[M_A - \bar{P}]$$

$$\rightarrow \quad Y_{4t} = \frac{i_A}{V_B} = \quad (q^2/h)\,[I-P]\,D^{-1}\,[I-B][M_B] \qquad = \quad (q^2/h)\,[M_A - \bar{P}]\,\bar{D}^{-1}\,[M_B - \bar{B}]$$

Semiclassical density of states is calculated from E(k) relation by noting that each state occupies a volume ($(2\pi/L)^d$ in k-space, d being the number of dimensions. Semiclassical dynamics from E(r,k) obtained from $\dfrac{d\vec{x}}{dt} = \dfrac{1}{\hbar}\vec{\nabla}_k E$, $\dfrac{d\vec{k}}{dt} = -\dfrac{1}{\hbar}\vec{\nabla}E$

If $E(\vec{x},\vec{k}) = \sum_j \dfrac{(\hbar k_j - qA_j(\vec{x}))^2}{2m} + U(\vec{x})$ ***where*** $q\vec{F} = -\vec{\nabla}U$ and $\vec{B} = \vec{\nabla}\,x\,\vec{A}$

Then, $\hbar\vec{v} = \dfrac{\hbar\vec{k} - q\vec{A}(\vec{x})}{m} \equiv \dfrac{\hbar\vec{k}'}{m}$, ***and*** $\dfrac{d(\hbar\vec{k}')}{dt} = q(\vec{F} + \vec{v}\;x\;\vec{B})$

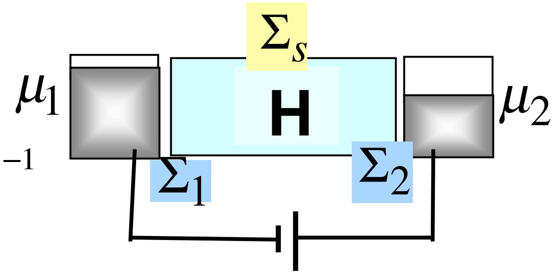
NEGF equations

"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:*** $g^{-1} = EI - \alpha - \beta g \beta^+$.

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

$$\Sigma \equiv \Sigma_s + \sum_j \Sigma_j, \quad \textbf{\textit{and}} \quad \Sigma^{in} \equiv \Sigma_s^{in} + \sum_j \Sigma_j^{in}$$

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. $i\hbar\, I_{op} = [HG^n - G^n H] + [\Sigma G^n - G^n \Sigma^+] + [G\Sigma^{in} - \Sigma^{in} G^+]$

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

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

$I_{Q,i} = \int dE\ (E - \mu_i)\, I_i(E)$ ***Energy absorbed per unit time from terminal 'i'***

4c. $I_i(E) = \dfrac{q}{h} \sum_j Trace[\Gamma_i G \Gamma_j G^+](f_i(E) - f_j(E))$ **(*used only if* Σ_s *is zero*)**

Including spin makes all matrices twice as big since each "grid point" has an up and a down component. ***Any quantity of interest can be obtained using the corresponding operator. For example, spin density*** = $Trace[G^n\vec{\sigma}]$***, spin current density*** = $Trace[I_{op}\vec{\sigma}]$ ***where*** $\vec{\sigma}$ is the Pauli spin matrix at the grid point of interest and zero elsewhere.

Pauli spin matrices: $\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix},\ \sigma_y = \begin{bmatrix} 0 & -i \\ +i & 0 \end{bmatrix},\ \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix},$ $\sigma_m \sigma_n = \delta_{mn} I + i\sum_p \varepsilon_{mnp}\sigma_p$

Eigenspinors: $+\hat{n} : \begin{Bmatrix} c \\ s \end{Bmatrix},\ -\hat{n} : \begin{Bmatrix} -s^* \\ c^* \end{Bmatrix},$ **where** $c \equiv \cos\dfrac{\theta}{2}\, e^{-i\varphi/2},\ s \equiv \sin\dfrac{\theta}{2}\, e^{+i\varphi/2}$

$\Sigma_j^{in} = \Gamma_j f_j$ ***, but*** Σ_s^{in} ***cannot in general be written as*** $\Gamma_s f_s$***, has to be calculated self-consistently . For elastic scatterers in equilibrium:*** $[\Sigma_s] = D\,[G]$, $[\Sigma_s^{in}] = D\,[G^n]$ ***(S)***

where $D = U_s\, U_s^*$ describes incoherent processes (or $D_{ijkl} = [U_s]_{ij}[U_s]^*_{kl}$) .

For inelastic scatterers, with dissipation occurring due to interaction with a reservoir with spectrum $D(+\varepsilon)$ for absorption and $D(-\varepsilon)$ for emission, replace (S) with

$$\left[\Sigma_s^{in}(E)\right] = D(+\varepsilon)\left[G^n(E-\varepsilon)\right] \quad \textbf{\textit{and}} \quad \left[\Gamma_s(E)\right] = D(+\varepsilon)\left[G^n(E-\varepsilon)\right] + D(+\varepsilon)\left[G^p(E+\varepsilon)\right]$$

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

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

$$\left[\Sigma_s^{in}(E)\right]_{ij} = D_{ik;jl}(+\varepsilon)\left[G^n(E-\varepsilon)\right]_{kl} \ \textbf{\textit{and}} \ \left[\Gamma_s(E)\right]_{ij} = D_{ijkl}(+\varepsilon)\left[G^n(E-\varepsilon)\right]_{kl} + D_{lkji}(+\varepsilon)\left[G^p(E+\varepsilon)\right]_{kl}$$

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

Scatterers in equilibrium with temperature T, then $\dfrac{D_{ijkl}(+\varepsilon)}{D_{lkji}(-\varepsilon)} = e^{-\varepsilon/k_B T}$

"Strong correlations" cannot be included in mean field treatment, need to start from ***multielectron Hamiltonian***. For example, for coupled quantum dots.

N=0:

$$H_0 = \begin{array}{c} 0 \\ \left[0\right] \end{array}$$

N=1:

$$H_1 = \begin{array}{c} \begin{array}{cccc} a & b & \bar{a} & \bar{b} \end{array} \\ \begin{bmatrix} \varepsilon_1 & t & 0 & 0 \\ t & \varepsilon_2 & 0 & 0 \\ 0 & 0 & \varepsilon_1 & t \\ 0 & 0 & t & \varepsilon_2 \end{bmatrix} \end{array}$$

N=2:

$$H_2 = \begin{array}{c} \begin{array}{cccccc} a\bar{a} & b\bar{b} & a\bar{b} & b\bar{a} & ab & \bar{a}\bar{b} \end{array} \\ \begin{bmatrix} 2\varepsilon_1 + U & 0 & t & t & 0 & 0 \\ 0 & 2\varepsilon_2 + U & t & t & 0 & 0 \\ t & t & \varepsilon_1 + \varepsilon_2 & 0 & 0 & 0 \\ t & t & 0 & \varepsilon_1 + \varepsilon_2 & 0 & 0 \\ 0 & 0 & 0 & 0 & \varepsilon_1 + \varepsilon_2 & 0 \\ 0 & 0 & 0 & 0 & 0 & \varepsilon_1 + \varepsilon_2 \end{bmatrix} \end{array}$$

N=3:

$$H_3 = \begin{array}{c} \begin{array}{cccc} b\bar{a}\bar{b} & a\bar{a}\bar{b} & ab\bar{b} & ab\bar{a} \end{array} \\ \begin{bmatrix} \varepsilon_1 + 2\varepsilon_2 + U & t & 0 & 0 \\ t & 2\varepsilon_1 + \varepsilon_2 + U & 0 & 0 \\ 0 & 0 & \varepsilon_1 + 2\varepsilon_2 + U & t \\ 0 & 0 & t & 2\varepsilon_1 + \varepsilon_2 + U \end{bmatrix} \end{array}$$

N=4:

$$H_4 = \begin{array}{c} ab\bar{a}\bar{b} \\ \left[2\varepsilon_1 + 2\varepsilon_2 + 2U\right] \end{array}$$

Law of Equilibrium: $\rho = \dfrac{1}{Z}\exp\left(-(H - \mu N)/k_B T\right)$

Expectation value of any quantity of interest obtained from corresponding operator.

For example, $\langle N \rangle = Trace(\rho N_{op})$