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/

General References: 1. Chapter 1, 4, 7.1, 8-11: Quantum Transport: Atom to Transistor 2. Lectures 1-5A, B: *http://www.nanohub.org/resources/5279* 3. Nanoelectronic Devices: A Unified View, *http://arxiv.org/abs/0809.4460v2*

A Brief Summary

Lectures 2-4: Conductivity

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

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

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

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

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

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

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

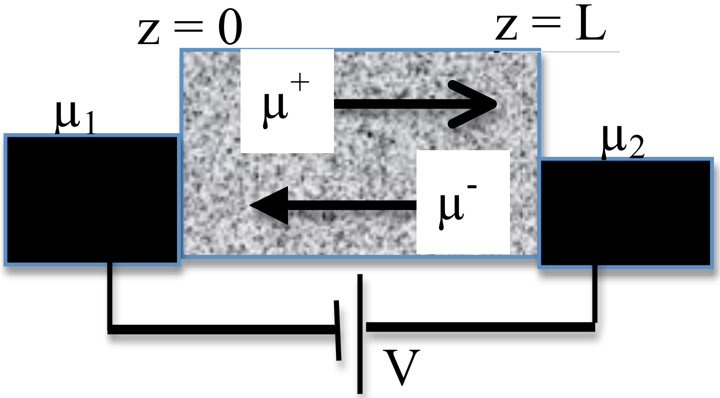
Linear Response: $$I \approx \int dE \left(-\frac{\partial f}{\partial E}\right) \tilde{I}(E)\,, \quad \Delta\mu << kT$$

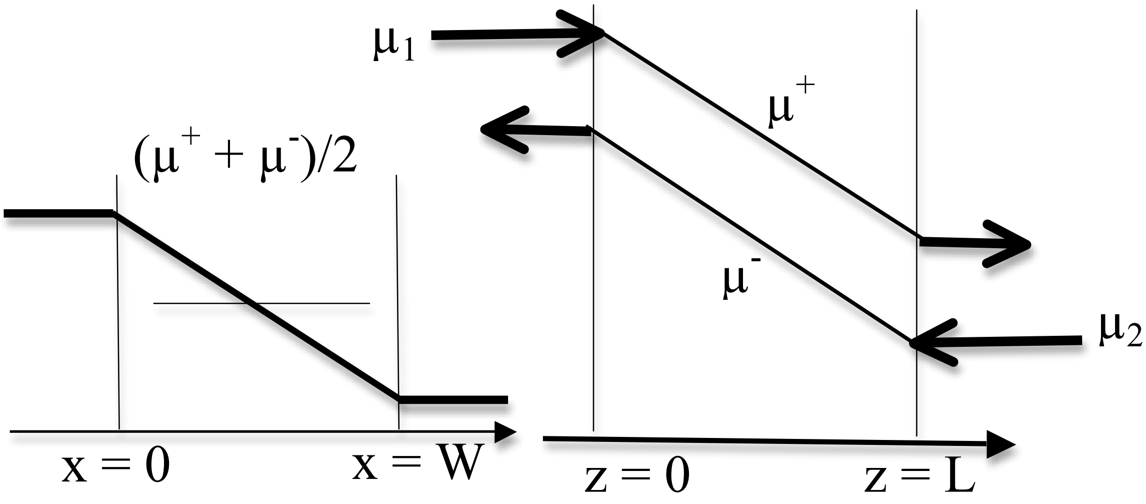
$$\tilde{I} \approx \quad q \frac{D(E)}{2L} v_z\,(\mu^+ - \mu^-) = \quad q^2 \, \frac{D(E)}{2L} \frac{v_z \lambda}{\lambda + L} \left(\frac{\mu_1 - \mu_2}{q}\right)$$

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

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

Lectures 5-7: Electrochemical Potential Profiles





Hall voltage (in x-direction):

$$V_H = \frac{2\omega_c W}{\pi v}\left(\frac{\mu^+ - \mu^-}{q}\right) \quad \rightarrow \quad \tilde{I} = q^2 \frac{D(E)}{WL}\frac{v^2}{d\omega_c} V_H$$

$$\begin{Bmatrix} V \\ V_H \end{Bmatrix} = \frac{1}{\tilde{\sigma}}\begin{bmatrix} L/W & -\omega_c\tau \\ +\omega_c\tau & W/L \end{bmatrix}\begin{Bmatrix} \tilde{I} \\ \tilde{I}_H \end{Bmatrix} \rightarrow \begin{Bmatrix} \tilde{I} \\ \tilde{I}_H \end{Bmatrix} \approx \tilde{\sigma}\begin{bmatrix} W/L & +\omega_c\tau \\ -\omega_c\tau & L/W \end{bmatrix}\begin{Bmatrix} V \\ V_H \end{Bmatrix}$$

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

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

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

Lectures 8-10: Scattering Theory of Transport

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

Two-probe conductance,

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

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

$$= (q^2/h)\,2\,[M-\bar{S}]\;[M+\bar{S}]^{-1}\,[M]$$

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

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

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

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

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

$$= (q^2/h)\,[M_A - \bar{P}]\,\bar{D}^{-1}\,[M_B - \bar{B}]$$

<u>Lectures 11-12,</u> ***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): $\frac{d\vec{x}}{dt} = \frac{1}{\hbar}\vec{\nabla}_k E$, $\frac{d\vec{k}}{dt} = -\frac{1}{\hbar}\vec{\nabla}E$

Assuming, $E(\vec{x},\vec{k}) = \sum_j \frac{(\hbar k_j - qA_j(\vec{x}))^2}{2m} + U(\vec{x})$

$$\rightarrow \quad v_i \equiv \frac{dx_i}{dt} = \frac{\hbar k_i - qA_i(\vec{x})}{m}, \qquad \hbar\frac{dk_i}{dt} = -\frac{\partial U}{\partial x_i} + q\sum_j v_j \frac{\partial A_j}{\partial x_i}$$

$$\frac{d}{dt}(\hbar k_i - qA_i(\vec{x})) = -\frac{\partial U}{\partial x_i} + q\sum_j v_j\left(\frac{\partial A_j}{\partial x_i} - \frac{\partial A_i}{\partial x_j}\right) = -\frac{\partial U}{\partial x_i} + q\sum_{j,n} v_j\,\varepsilon_{ijn}\left(\vec{\nabla}\,x\,\vec{A}\right)_n$$

$$\rightarrow \quad \hbar\vec{v} = \frac{\hbar\vec{k} - q\vec{A}(\vec{x})}{m} \equiv \frac{\hbar\vec{k}'}{m},$$

$$\frac{d(\hbar\vec{k}')}{dt} = q(\vec{F} + \vec{v}\;x\;\vec{B}) \qquad \text{where} \quad q\vec{F} = -\vec{\nabla}U \;\text{ and } \vec{B} = \vec{\nabla}\,x\,\vec{A}$$

Cyclotron Frequency: $\hbar^2\frac{d}{dE}A(k') = qBT \quad \rightarrow \quad \frac{T}{2\pi} = \frac{1}{\omega_c} = \frac{1}{qB}\frac{\hbar^2}{2\pi}\frac{dA(k')}{dE}$

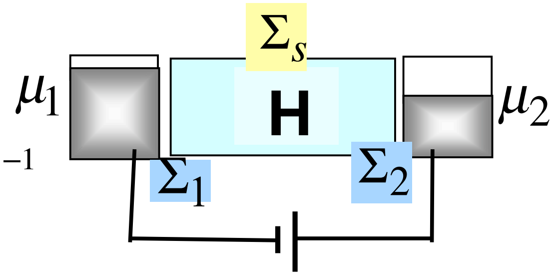
Lectures 13-23: NEGF equations

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

$$\Gamma_j = i[\Sigma_j - \Sigma_j^+]\,,\ \Gamma_s = i[\Sigma_s - \Sigma_s{}^+]$$

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

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

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'***

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)***

$\Sigma_j^{in} = \Gamma_j f_j$ ***, 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:***

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

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

Lectures 24-32: Spin

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, (per unit energy) spin density =*** $Trace[G^n\vec{\sigma}]/2\pi$***, spin current***

density = $Trace[I_{op}\vec{\sigma}]/2\pi$ ***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** $c \equiv \cos\frac{\theta}{2}\, e^{-i\varphi/2}, \ s \equiv \sin\frac{\theta}{2}\, e^{+i\varphi/2}$

Lectures 33-37: Energy exchange

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

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

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

(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)

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

$$\left[\Gamma_s(E)\right]_{ij} = D_{ijkl}(+\varepsilon)\left[G^n(E-\varepsilon)\right]_{kl} + D_{lkji}(+\varepsilon)\left[G^p(E+\varepsilon)\right]_{kl}$$

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

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

Lectures 38-43: Strong correlations

"Strong correlations" cannot be included in mean field treatment, need to start from ***multiparticle Hamiltonian*** H: For ***equilibrium*** problems use $\rho = \frac{1}{Z}\exp\left(-(H-\mu N)/k_B T\right)$. Expectation value of any quantity of interest obtained from corresponding operator. For example, $\langle N \rangle = Trace(\rho N_{op})$

For non-equilibrium problems can use rate equations in multiparticle or Fock space, but no standard method for including broadening.