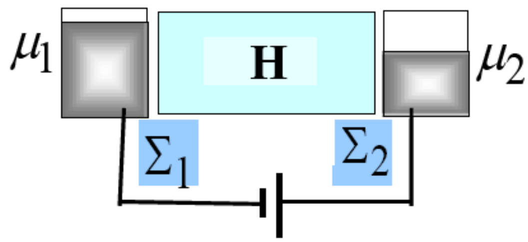
HW#4: Problems 5-7, Due Monday March 2, 2009 in class

Please remember to turn in a copy of your MATLAB codes for all numerical problems.

Coherent transport



$\Gamma_1 = i[\Sigma_1 - \Sigma_1^+], \Gamma_2 = i[\Sigma_2 - \Sigma_2^+]$

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

2. $A(E) = i[G - G^+] = G\Gamma_1 G^+ + G\Gamma_2 G^+$ *Density of states * 2π*

3. $[G^n(E)] = [G\Gamma_1 G^+]\ f_1 + [G\Gamma_2 G^+]\ f_2$ *Electron density * 2π*

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

4b. $I(E) = \frac{q}{h}\ Trace[\Gamma_1 G \Gamma_2 G^+](f_1(E) - f_2(E))$ *2-terminal current/energy*

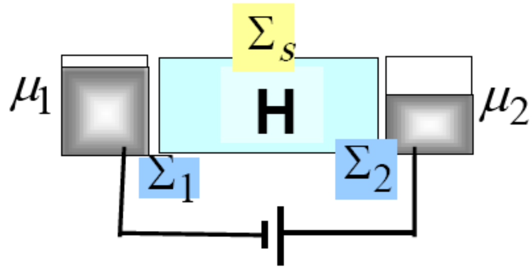
(1 x 1) version

3: $n(E) = D(E)\frac{\gamma_1 f_1(E) + \gamma_2 f_2(E)}{\gamma_1 + \gamma_2}$ *Electron density*

4a. $I_i(E) = \frac{q}{\hbar}\gamma_i\left(D(E) f_i(E) - n(E)\right)$ *Current/energy at terminal 'i'*

4b. $I(E) = \frac{q}{\hbar}\frac{\gamma_1\gamma_2}{\gamma_1 + \gamma_2} D(E)(f_1(E) - f_2(E))$ *2-terminal current/energy*

Incoherent transport



$$\Gamma_1 = i[\Sigma_1 - \Sigma_1^+], \Gamma_2 = i[\Sigma_2 - \Sigma_2^+], \Gamma_s = i[\Sigma_s - \Sigma_s^+]$$

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

$$where \quad [\Sigma_s] = D[G]$$

2. $A(E) = i[G - G^+]$

3. $[G^n(E)] = [G\Gamma_1 G^+]\ f_1 + [G\Gamma_2 G^+]\ f_2 + [G\Sigma_s^{in} G^+]$

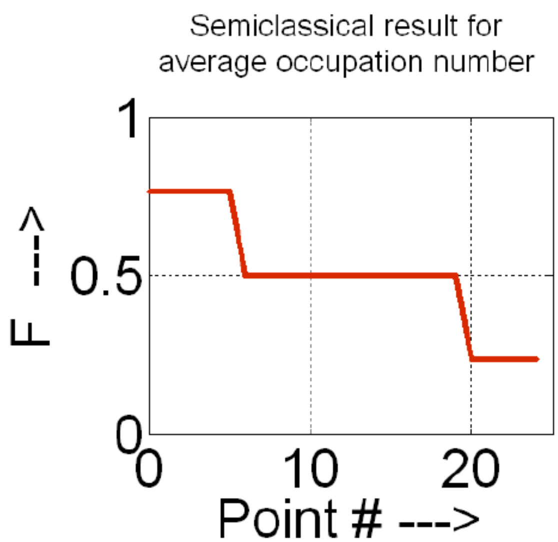
$$where \quad \left[\Sigma_s^{in}\right] = D\left[G^n\right]$$

4b. $I_i = \frac{q}{h} \int dE\, (Trace[\Gamma_i A]\ f_i - Trace[\Gamma_i G^n])$, *i: Terminals*

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

Problem 5: For each of problems 3, 4 plot the average occupation number defined as $F(i) \equiv G^n(i,i)/A(i,i)$ across the conductor at an energy E = 0.5 eV. Compare the result from problem 4 with semiclassical one.

(Hint: For semiclassical result, consider an individual scatterer separately and calculate T(E) and R(E)=1-T(E) from the formula given in problem 2-(c). Then cascade two scatterers to calculate $f^+(i), f^-(i)$ across the conductor and finally get the average occupation number defined as $F(i)_{semiclassical} \equiv \dfrac{f^+(i)+f^-(i)}{2}$).



Problem 6: For a semi-infinite contact with a Hamiltonian $\begin{bmatrix} \alpha & \beta & 0 & \cdots & \cdots \\ \beta^+ & \alpha & \beta & \cdots & \cdots \\ 0 & \beta^+ & \alpha & \beta & \cdots \\ \cdots & \cdots & \cdots & \cdots & \\ \cdots & \cdots & \cdots & \cdots & \end{bmatrix}$

the ***surface Green's function*** satisfies the equation $g = [(E+i0^+)I-\alpha-\beta g\beta^+]^{-1}$

For $\alpha = 2t_0$, $\beta = -t_0$ (t_0 being a number),

show that $g = -e^{ika}/t_0$ where $E+i0^+ = 2t_0(1-\cos ka)$.

Problem 7. Conductance quantization: Consider a uniform two-dimensional conductor of width equal to 8 nm.

(a) Using a discrete lattice with points spaced by 0.5 nm plot the transmission T(E) versus energy E (-0.1 < E < +0.5 eV), assuming an effective mass appropriate for GaAs, m = 0.07*9.1e-31 Kg.

To obtain the contact self-energies, use two different methods to evaluate the surface Green's function: (a) Iterative solution of $g = [(E + i0^+)I - \alpha - \beta g \beta^+]^{-1}$ and (b) basis transformation into transverse modes each of which has g = $-(1/t_0)\exp(+ika)$.

(b) The transmission should show a series of steps at different values of the energy as new modes start conducting. Compare the energies at which these steps occur with the analytical values for the transverse mode energies calculated using both parabolic and cosine dispersion relations.

(c) Plot the local density of states across the width of the conductor at an energy of E = 0.5 eV.

(d) Repeat parts (a) and (c) with a single delta function scatterer of strength 10 eV–nm^2 located at the center of the conductor.