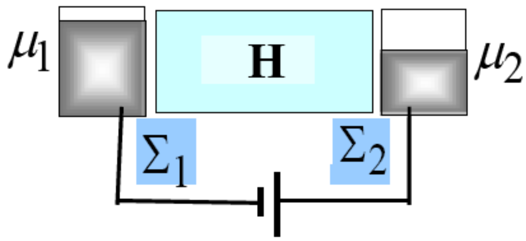
HW#3: Problems 1-4, Due Wednesday February 25, 2009 in class

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

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

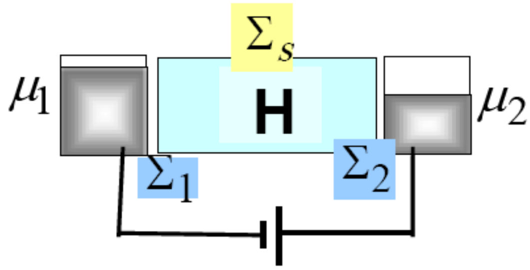
(1 x 1) version

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

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

4b. $I(E) = \dfrac{q}{\hbar}\dfrac{\gamma_1\gamma_2}{\gamma_1 + \gamma_2} D(E)(f_1(E) - f_2(E))$ *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 1: The objective of this problem is to write a MATLAB code to describe numerically the propagation of a wavepacket and show that it travels with a velocity equal to the group velocity $(1/\hbar)\ dE/dk$. Consider a discrete lattice with points spaced by a = 2e-10 m extending from –2e-8 m to + 2e-8 m, described by a Hamiltonian matrix with non-zero elements given by ($t_0 = \hbar^2 / 2ma^2$, m: free electron mass)

$$H_{ii} = 2t_0,\ H_{i,i+1} = H_{i,i-1} = -t_0$$

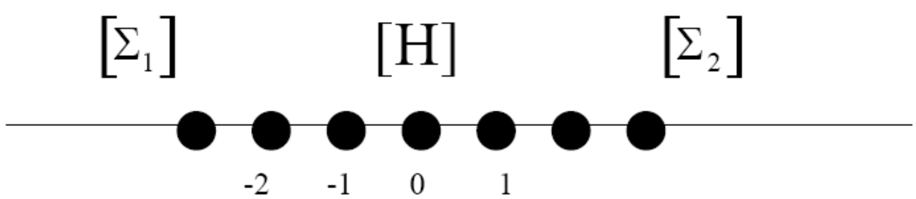
Assume that the initial wavefunction is given by $\psi(z, t=0) = e^{+ikz}\, e^{-(z/20a)^2}$, where $k = \pi/4a$ and plot the center of the wavefunction

$$\langle z(t)\rangle = \frac{\int dz\, z\, |\psi(z,t)|^2}{\int dz\, |\psi(z,t)|^2}$$

as a function of time. Compare the velocity $d\langle z(t)\rangle / dt$ with the group velocity

$$(1/\hbar)\ dE/dk = \quad (2at_0/\hbar)\sin ka$$

Problem 2: Consider a 1-D wire



modeled with a Hamiltonian having $H_{n,n} = +2t_0$, $H_{n,n+1} = -t_0 = H_{n,n-1}$ (all other elements are zero), such that the dispersion relation is given by $E = 2t_0(1-\cos ka)$. Use t_0 = 1 eV. For a lattice with Np points, you could set up the H matrix using the command

H = - t0*diag(ones(1,Np-1),1) - t0*diag(ones(1,Np-1),-1)+2t0*diag(ones(1,Np));

Σ_1 is a matrix with all zeroes except for $\Sigma_1(1,1) = \sigma$, while Σ_2 has all zeroes except for $\Sigma_2(Np, Np) = \sigma$.

(a) Using $\sigma(E) = -t_0\, e^{+ika}$, plot numerically the transmission T(E) over the energy range -.5 eV < E < +4.5 eV, using Np = 25.

(b) Consider the same 1-D wire with Np=25 points and with one point scatterer located in the middle. This is accomplished by setting H(13,13) = U+2*t0 (rest of H same as before).

(a) Using $\sigma(E) = -t_0\, e^{+ika}$ and U = 1 eV, plot numerically the transmission T(E) over the energy range 0 eV < E < 1 eV.

(c) Using $\sigma(E) = -t_0\, e^{+ika}$, show analytically that $T(E) = \dfrac{1}{1+(U/2\,t_0 \sin ka)^2}$ and compare this result with the numerical result from part (b).

Hint: Treat point "13" of the lattice as the channel described by a (1x1) Hamiltonian and the rest of the wire on each side as Σ_1 and Σ_2.

Note: This problem is similar to Prob. 1, 2 of HW#8 from ECE 495N, Fall 2008. Both homeworks and solutions are posted at http://sites.google.com/site/ece495n/

You are welcome to look at the solutions but what you submit should be your own work.

Problem 3: Consider the same 1-D wire with Np=25 points with two point scatterers located one near each end: H(6,6) = U+2*t0, H(20,20) = U+2*t0 (rest of H same as before). Using $\sigma(E) = -t_0\, e^{+ika}$ and U = 1 eV, plot numerically the terminal currents versus energy over the range 0.1 eV< E < 1 eV, assuming $f_1 = 1,\ \ f_2 = 0$.

Problem 4: Consider the same device as in Problem 3 but with phase-breaking processes described by D = $5\times10^{-2}eV^2$. Use the equations for incoherent transport to plot the terminal currents versus energy from Eq.(4b), with $f_1 = 1,\ \ f_2 = 0$. Note that Eq.(4a) is not valid for incoherent transport. Also, both Eqs.(1) and (3) have to be solved self-consistently.