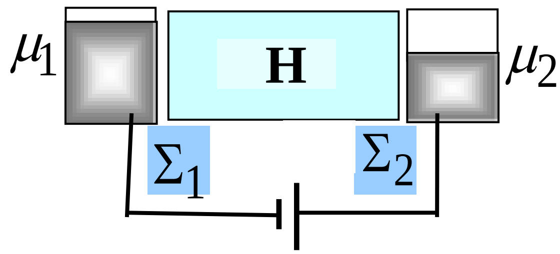
ECE 495N, Fall'08 ME118, MWF 1130A – 1220P

HW#8: Due Wednesday Dec.3 in class.

Basic equations of coherent transport



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

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

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

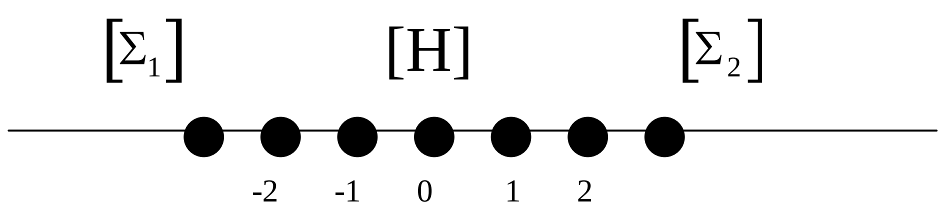
$$[G^{n}(E)] = [G\Gamma_1 G^{+}]\ f_1 + [G\Gamma_2 G^{+}]\ f_2$$ ***Electron density***

$$I_i(E) = \frac{q}{h}((Trace[\Gamma_i A])\ f_i - Trace[\Gamma_i G^{n}])$$ ***Current/energy***

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

In general H has to be replaced with H+U, where U has to be calculated self-consistently from an appropriate "Poisson"-like equation, but you can ignore this aspect in the following problem.

Problem 1: Consider a 1-D wire



modeled with a Hamiltonian having $H_{n,n+1} = -t_0 = H_{n,n-1}$ (all other elements are zero), such that the dispersion relation is given by $E = -2t_0 \cos ka$. 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);

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 $\sigma = -i(1eV)/2$ and Np = 5, plot numerically the transmission $T(E) = Trace[\Gamma_1 G \Gamma_2 G^+]$ over the energy range -2.5 eV < E < +2.5 eV and compare the peaks in the transmission with the eigenvalues of [H].

(b) Using $\sigma(E) = -t_0\, e^{+ika}$, plot numerically the transmission T(E) over the energy range -2.5 eV < E < +2.5 eV, using Np = 5 and Np = 10.

(c) Using $\sigma(E) = -t_0\, e^{+ika}$, show analytically that the transmission is equal to one over the energy range $-2t_0 < E < +2t_0$. Hint: Treat one point 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.

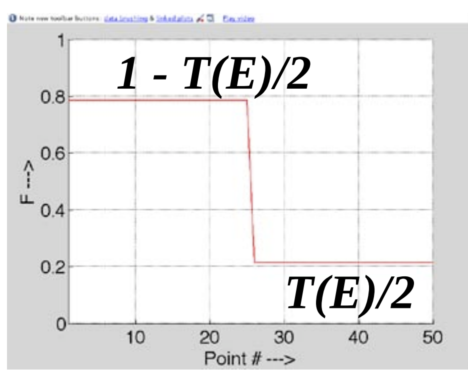
Problem 2: Consider the same 1-D wire with Np=50 points and with one point scatterer located in the middle. This is accomplished by setting H(25,25) = U (rest of H same as before). (a) Using $\sigma(E) = -t_0\, e^{+ika}$ and U = 2 eV, plot numerically the transmission T(E) over the energy range -2 eV < E < +2 eV.

(b) Using $\sigma(E) = -t_0\, e^{+ika}$, show analytically that $T(E) = \dfrac{1}{1 + (U/2t_0 \sin ka)^2}$.

Hint: Treat point "25" 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.

(c) Compare the numerical result from part (a) with the analytical result from part (b).

Problem 3: Consider the same 1-D wire from Problem 2 with Np=50 points and one point scatterer, U = 2 eV. At an energy E = -1 eV, assuming f_1=1, f_2=0, plot numerically the quasi-Fermi level defined as $F(i) \equiv G^n(i,i)/A(i,i)$ and compare with the semiclassical result that we discussed in class, shown on the right.



Semiclassical result for quasi-Fermi level.