ECE 659: Quantum Transport Spring 2009

EE 117, MWF 930A-1020P

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

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

Midterm exam: Monday, 3/9
Covering Weeks 1-7: Semiclassical and Quantum transport
Closed book, notes (see last 4 pages) will be provided

General References

1. Chapter 1, 7.1, 8, 9, 11.1, 11.2: Quantum Transport: Atom to Transistor
2. Lectures 1A, B and 2A, B : *http://www.nanohub.org/resources/5279*
3. Nanoelectronic Devices: A Unified View, *http://arxiv.org/abs/0809.4460v2*

There will be five questions on the midterm exam. The homework problems (without the MATLAB implementation) are a good guide. In addition the following problems are intended to help you prepare. Solutions will be posted.

Problem 1: A conductor has a single band with an isotropic E(k) relation of the form $E = Ak^{\alpha}$, where A and α are constants. Show that at low temperatures (for which $-\partial f / \partial E$ can be approximated by a delta function at E = µ), irrespective of A and α, we can write for the sheet conductivity and the Hall resistance

(a) $\sigma_{zz} = q^2\, n_s\, \tau / m$, if m is defined as $\hbar k / v$ evaluated at E = µ.

and (b) $R_H = \omega_c \tau / \sigma_{zz} = B / q n_s$

where n_s is the electron density per unit area.

Problem 2: A conductor with M modes has one point scatterer having a scattering matrix of the form $\begin{Bmatrix} I_1^- \\ I_2^- \end{Bmatrix} = \begin{bmatrix} R & T \\ T & R \end{bmatrix} \begin{Bmatrix} I_1^+ \\ I_2^+ \end{Bmatrix} = \frac{q}{h} M \begin{bmatrix} R & T \\ T & R \end{bmatrix} \begin{Bmatrix} \mu_1^+ \\ \mu_2^+ \end{Bmatrix}$

with R+T = 1 (‘+’ denotes incoming flux, ‘-‘ denotes outgoing flux).

(a) Assuming $\mu_1^+ = qV$ and $\mu_2^+ = 0$, show that the average normalized electrochemical potential defined by $(\mu^+ + \mu^-)/2qV$ has the profile shown below and label the plateaus in the profile. What is the current $(I^+ - I^-)$?

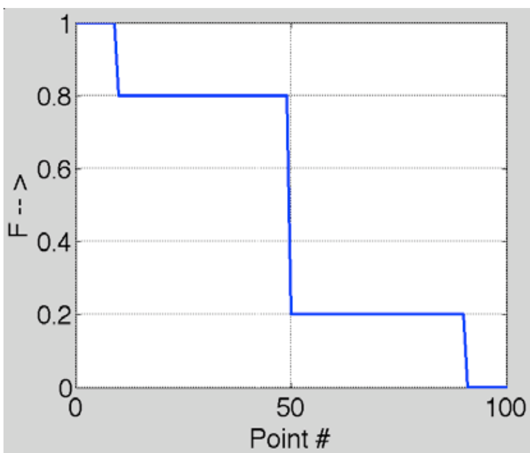
(b) Now consider the same conductor but with two identical point scatterers, each having a scattering matrix with a transmission T. Label the plateaus in the average normalized electrochemical profile shown. What is the current $(I^+ - I^-)$?

(c) The electrochemical potential profile suggests that in part (a) we have three localized resistances, one associated with the scatterer and two associated with the interfaces. Divide the drop in potential across each of these by the current to obtain the magnitude of these resistances (normalized to $h/q^2 M$).

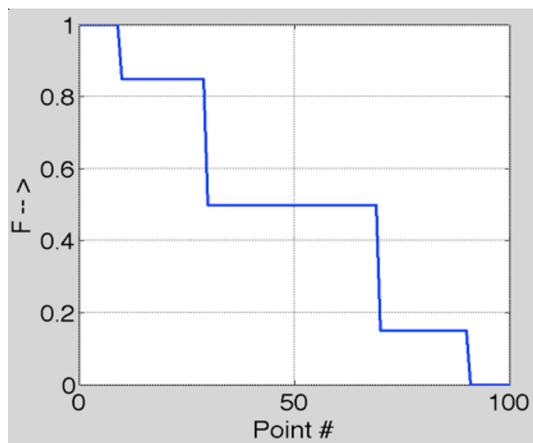
(d) Compare the scatterer resistance (for the conductor with one scatterer) with what you obtain using the relation discussed in class: $Y = (q^2/h)\, 2\, [M - \bar{S}]\, [M + \bar{S}]^{-1}\, [M]$

(e) For part (b), obtain the four resistances associated with the two scatterers and the two interfaces.

One scatterer



Two scatterers



Problem 3: Consider a junction between two conductors having M_1 and M_2 modes respectively ($M_1 > M_2$) described by a scattering matrix of the form

$$\begin{Bmatrix} I_1^- \\ I_2^- \end{Bmatrix} = \begin{bmatrix} (M_1 - M_2)/M_1 & 1 \\ M_2/M_1 & 0 \end{bmatrix} \begin{Bmatrix} I_1^+ \\ I_2^+ \end{Bmatrix} = \frac{q}{h} \begin{bmatrix} (M_1 - M_2) & M_2 \\ M_2 & 0 \end{bmatrix} \begin{Bmatrix} \mu_1^+ \\ \mu_2^+ \end{Bmatrix}$$

Assuming $\mu_1^+ = qV$ and $\mu_2^+ = 0$,

(a) show that the average normalized electrochemical potential defined by $(\mu^+ + \mu^-)/2qV$ has the same profile as in Problem 2a and label the plateaus in the profile.

(b) Find the current and each of the three resistances associated with the two interfaces and the junction respectively.

(c) Compare the junction resistance with what you obtain using the relation discussed in class: $Y = \quad (q^2/h)\, 2\, [M - \bar{S}]\, [M + \bar{S}]^{-1}\, [M]$

Problem 4: A 2-D conductor is described by a Hamiltonian of the form

$$H = \frac{(p_x - qA_x)^2}{2m} + \frac{(p_y - qA_y)^2}{2m}$$

where the vector potential $\vec{A} = \hat{x}A_x + yA_y$ is constant in space. Find the dispersion relation $E(k_x, k_y)$ assuming a wavefunction of the form $\psi \sim \exp(i\vec{k}.\vec{r})$?

Problem 5: We wish to model the 2D conductor in Problem 4 with a discrete square lattice having a nearest neighbor Hamiltonian whose non-zero elements are

$$H_{n,m} = \varepsilon \;\; if \;\; \vec{d}_m = \vec{d}_n$$

$$H_{n,m} = -t_x \exp(-i\phi_x) \;\; if \;\; \vec{d}_m - \vec{d}_n = \hat{x}a \qquad H_{n,m} = -t_x \exp(+i\phi_x) \;\; if \;\; \vec{d}_m - \vec{d}_n = -\hat{x}a$$

$$H_{n,m} = -t_y \exp(-i\phi_y) \;\; if \;\; \vec{d}_m - \vec{d}_n = \hat{y}a \qquad H_{n,m} = -t_y \exp(+i\phi_y) \;\; if \;\; \vec{d}_m - \vec{d}_n = -\hat{y}a$$

All other elements are zero. Find the dispersion relation assuming a wavefunction of the form $\psi \sim \exp(i\vec{k}.\vec{d}_m)$. How would you choose $\varepsilon, t_x, \phi_x, t_y$ $and\, \phi_y$ so as to match the dispersion relation from Problem 4 for small energy E ?

Problem 6: Consider a device with two terminals described by (1x1) matrices: H = [ε], $\Sigma_1 = [-i\gamma_1/2]$ and $\Sigma_2 = [-i\gamma_2/2]$.

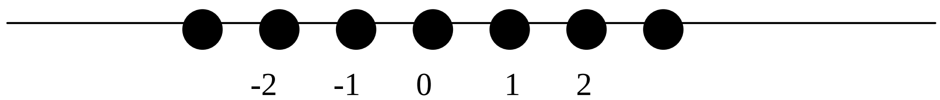
(a) Starting from the general NEGF equations for coherent transport, show that

$$G^n(E) = A(E)\frac{\gamma_1 f_1(E) + \gamma_2 f_2(E)}{\gamma_1 + \gamma_2}$$

$$I_1(E) = -I_2(E) = \frac{q}{h}\frac{\gamma_1\gamma_2}{\gamma_1 + \gamma_2} A(E)(f_1(E) - f_2(E))$$

(b) Now show that these equations remain unchanged even if we include incoherent processes through a non-zero D.

Problem 7: A uniform wire is modeled as a discrete lattice with points spaced by ‘a’



having a Hamiltonian with $H_{n,n} = 2t_0$ and $H_{n,n+1} = -t_0 = H_{n,n-1}$ (all other elements are zero), such that the dispersion relation is given by $E = 2t_0(1-\cos ka)$. The two ends are connected to two contacts with Fermi functions f_1 and f_2.

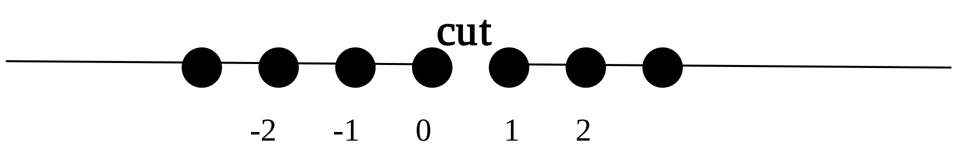
(a) What is the local density of states at the point “0”, $D(0,E) = A(0,0;E)/2\pi$? Hint: Treat the point “0” as the channel and represent the wire on either side through self-energies.

(b) Starting from the general NEGF equations for coherent transport, show that

$$G^n(0,0;E) \quad = \quad A(0,0;E)\,\frac{f_1(E)+f_2(E)}{2}$$

$$I_1(E) = -I_2(E) = \frac{q}{h}\left(f_1(E)-f_2(E)\right), \qquad \textbf{\textit{for}}\ 0 < E < 4t_0$$

(c) Suppose we cut the wire in Part (a) into two separate semi-infinite wires as shown so that $H_{01} = H_{10} = 0$ (other elements of the H-matrix remain unchanged).



What is the local density of states at the point “0”, D(0,E) ? What is the current ?

Problem 8: Consider a conductor with a single band (with two degenerate spins) with an isotropic E(k) relation of the form $E = Ak^{\alpha}$, where A and α are constants. Show that at low temperatures (for which $-\partial f/\partial E$ can be approximated by a delta function at E = μ), irrespective of A and α, the ballistic conductance $G_{ballistic} = (2q^2/h)M$, where $M = \sqrt{2n_s/\pi}\,W$ for a 2D conductor of width W and $M = \left(3\pi^2 n\right)^{2/3} S/4\pi$ for a 3D conductor with a cross-section S.

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Notes on Lectures 2-20: Semiclassical and Quantum Transport

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

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

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

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

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

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

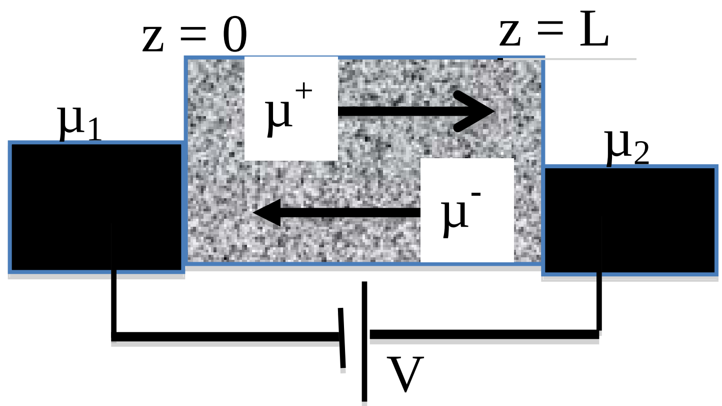
$$\tilde{I} \approx q\frac{D(E)}{2L}v_z(\mu^+ - \mu^-) = q^2\frac{D(E)}{2L}\frac{v_z\lambda}{\lambda+L}\left(\frac{\mu_1-\mu_2}{q}\right)$$

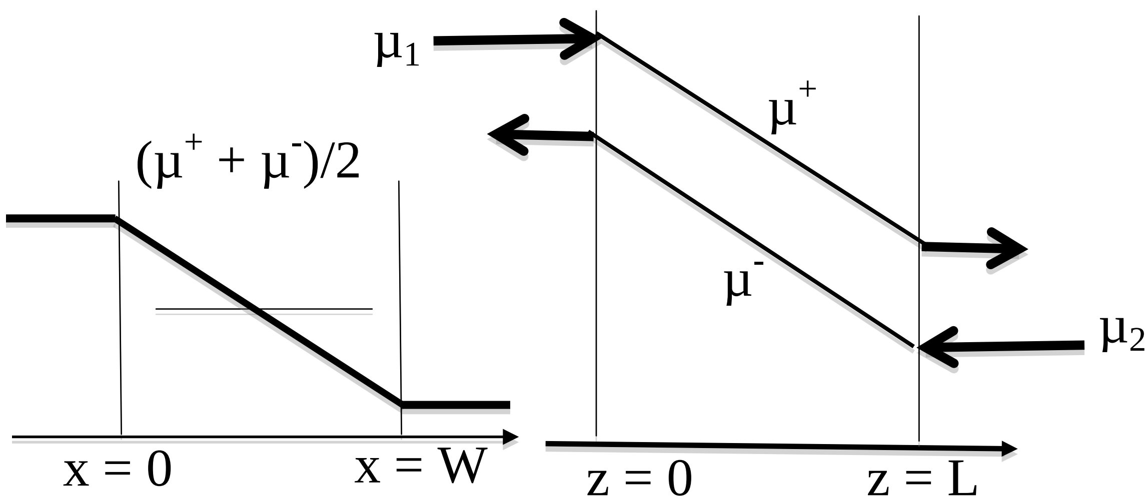
$$= \underbrace{q^2\frac{D(E)}{WL}\frac{v^2\tau}{d}}_{\equiv\tilde{\sigma}(E)}\frac{W}{\lambda+L}V \qquad \textit{\textbf{(d=2 for 2D, 3 for 3D)}}$$

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

__Lectures 5-7:__ Electrochemical

Potential Profiles





Hall voltage (in x-direction):

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

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

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

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

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

Lectures 8-10: *Scattering Theory of Transport*

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

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

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

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

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

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

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

Lectures 11-12, 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 $E(\vec{r},\vec{k})$: $\dfrac{d\vec{x}}{dt} = \dfrac{1}{\hbar}\vec{\nabla}_k E$, $\dfrac{d\vec{k}}{dt} = -\dfrac{1}{\hbar}\vec{\nabla}E$

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

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

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

$$\rightarrow \vec{v} = \frac{\hbar\vec{k} - q\vec{A}(\vec{x})}{m} = \frac{\hbar\vec{k}'}{m}, \qquad \frac{d(\hbar\vec{k}')}{dt} = q(\vec{F} + \vec{v}\times\vec{B})$$

where $q\vec{F} = -\vec{\nabla}U$ and $\vec{B} = \vec{\nabla}\times\vec{A}$

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

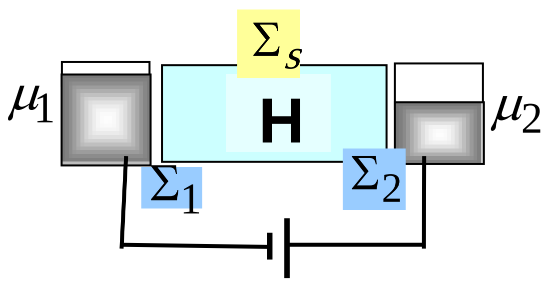
Lectures 13-20, Quantum Transport: *The NEGF equations for elastic (but not necessarily coherent) transport, with all dissipation limited to contacts. Inelastic transport with dissipation in channel to be discussed later in the course.*

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

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

$$\Sigma \equiv \Sigma_s + \sum_j \Sigma_j,$$

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



Note: $\Sigma_j^{in} = \Gamma_j f_j$***, but*** Σ_s^{in} ***cannot in general be written as*** $\Gamma_s f_s$.

Instead it has to be calculated self-consistently from $[\Sigma_s] = D[G]$, $[\Sigma_s^{in}] = D[G^n]$

where D describes incoherent processes (has nothing to do with density of stets D(E)).

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

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

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

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