ECE 659 Spring '09

HW#2, Due Wednesday February 11, 2009 in class

Weeks 1-3: Semiclassical Transport, Summary

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

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

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

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

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

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

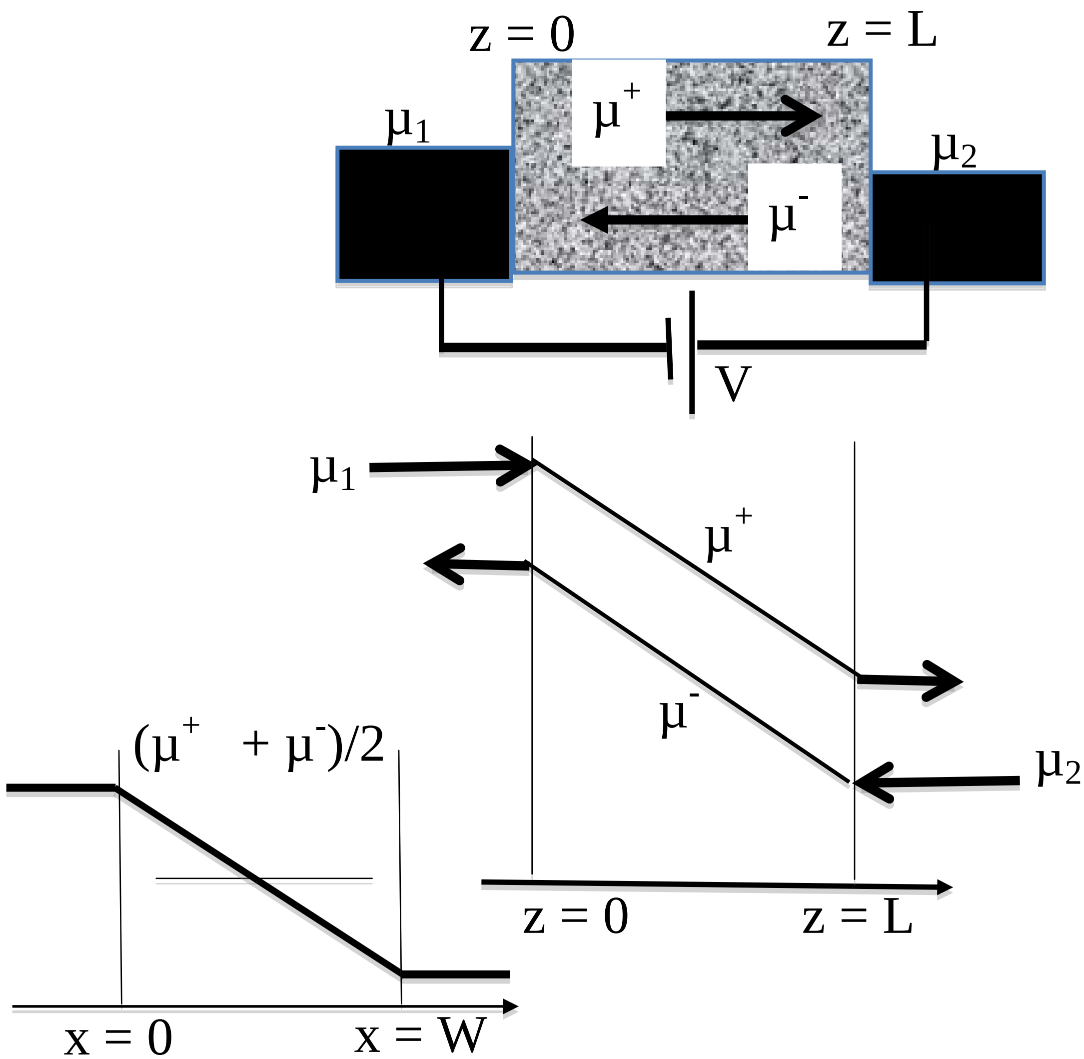
$$f^+(z,E) - f^-(z,E) = \frac{\lambda}{\lambda + L}(f_1(E) - f_2(E))$$

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

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

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

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



Hall voltage (in x-direction):

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

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

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

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).

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

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

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

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

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

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

Semiclassical dynamics from $E(\vec{r},\vec{k})$***:***

$$\frac{d\vec{x}}{dt} = \frac{1}{\hbar}\vec{\nabla}_k E\ ,\quad \frac{d\vec{k}}{dt} = -\frac{1}{\hbar}\vec{\nabla}E$$

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

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

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

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

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

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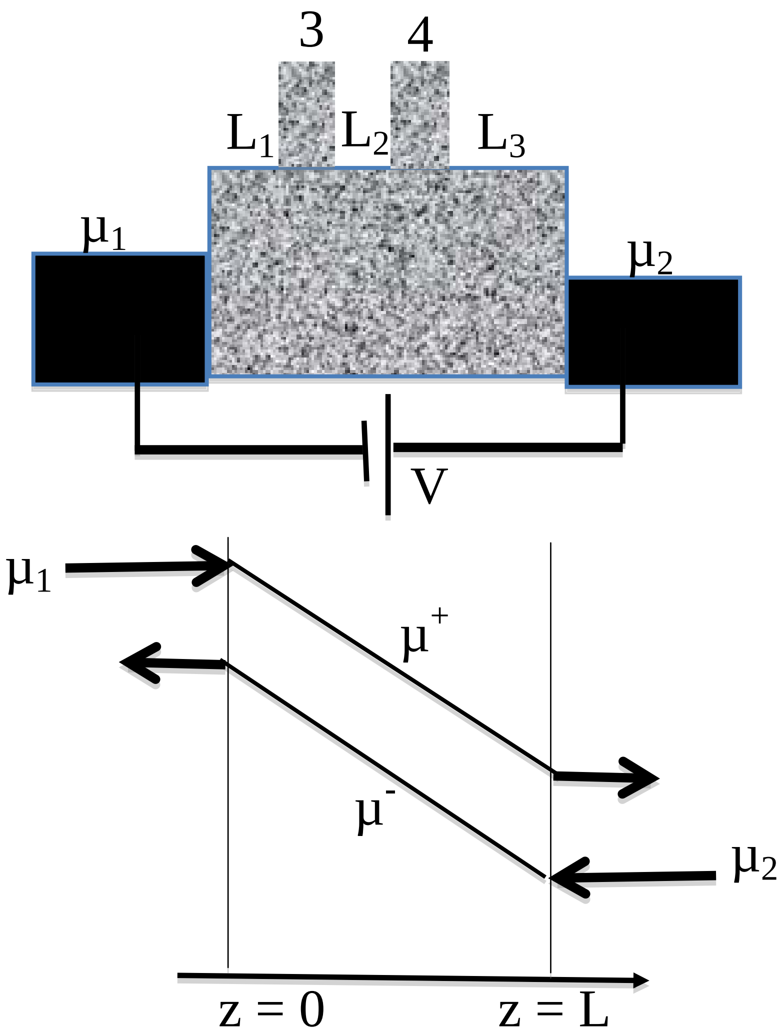
1. Consider a four-probe structure as shown below with $L = L_1 + L_2 + L_3$ and assume that the voltage probes 3 and 4 are non-invasive. What is the ratio $\frac{R_{4pt}}{R_{2pt}} = \frac{\mu_3 - \mu_4}{\mu_1 - \mu_2}$, (a) if the voltage probes float to the local average electrochemical potential, $(\mu^+ + \mu^-)/2$? (b) if probe 3 floats to μ^- and probe 4 floats to μ^+?



2. Suppose the four-probe structure in Problem 1 has an S-matrix of the form

$$\bar{S} = [S][M] = \begin{bmatrix} r_1 & t' & a' & c' \\ t & r_2 & b' & d' \\ a & b & r_3 & 0 \\ c & d & 0 & r_4 \end{bmatrix}$$

with the reflection coefficients $r_{1,2,3,4}$ determined by the requirement that the first two columns add up to M_A and the last two columns to M_B. Probes 1 and 2 represent current probes while 3 and 4 represent voltage probes.

Note that sum rules require the followings.
$$\begin{cases} a' + b' = a + b \\ c' + d' = c + d \\ a' + c' + t' = a + c + t \\ b' + d' + t = b + d + t' \end{cases}$$

(a) Show that $1/R_{2pt} = t + \dfrac{ab'}{a+b} + \dfrac{cd'}{c+d} = t' + \dfrac{a'b}{a+b} + \dfrac{c'd}{c+d}$

$$R_{4pt} = \quad R_{2pt} \frac{ad - bc}{(a+b)(c+d)}$$

For an example of the use of these results to interpret experiments you could look at Gao et al., Phys. Rev. Lett. vol.95, 196802 (2005), see Eq.(3).

(b) Assuming $a = a' = \dfrac{K\lambda}{\lambda + L_1}$, $b = b' = \dfrac{K\lambda}{\lambda + L_2 + L_3}$, $c = c' = \dfrac{K\lambda}{\lambda + L_1 + L_2}$, $d = d' = \dfrac{K\lambda}{\lambda + L_3}$

and $t = t' = \dfrac{\lambda}{\lambda + L}$ with $L = L_1 + L_2 + L_3$, show that $R_{2pt} \approx L/\lambda$ and $R_{4pt} \approx L_2/\lambda$ for small K.

(c) Plot numerically the two-terminal resistance R_{2pt} and the four-terminal resistance R_{4pt} versus log(K), assuming $L_1 = 100\lambda$, $L_2 = 20\lambda$, $L_3 = 200\lambda$, for 1e-3 < K < 1.

3. Consider a 2-D material like graphene having

$$E(\vec{x},\vec{k}) = v_f \left|\hbar\vec{k} - q\vec{A}\right| + U(\vec{x}) .$$

Starting from the equations for semiclassical dynamics $\frac{d\vec{x}}{dt} = \frac{1}{\hbar}\vec{\nabla}_k E$, $\frac{d\vec{k}}{dt} = -\frac{1}{\hbar}\vec{\nabla} E$

obtain expressions for $\frac{d\vec{x}}{dt}$ and $\frac{d(\hbar\vec{k} - q\vec{A})}{dt}$ and show that they agree with the usual result for parabolic bands with $E(\vec{x},\vec{k}) = (\hbar\vec{k} - q\vec{A})^2 / 2m + U(\vec{x})$

if we define mass as $m = \left|\hbar\vec{k} - q\vec{A}\right| / \left|\vec{v}\right| = (E-U)/v_f^{\,2}$.

4. In HW 1, we tried to find an expression for mobility for arbitrary temperature. It is simpler to focus on low temperatures for which $\left(-\frac{\partial f}{\partial E}\right) \simeq \delta(E - E_f)$ and all conductivities are determined by a single energy $E = E_f$:

$$\sigma_{zz}(E) = q^2 \frac{D(E)}{WL}\frac{v^2\tau}{d}$$

$$\rho_{zx}(E) = \frac{\omega_c \tau}{\sigma_{zz}(E)}$$

(a) Show that $\rho_{zx} = \frac{B}{qn}$ in both 2D and 3D.

Note : (1) At low temperatures, $n = \frac{\left|\vec{k} - q\vec{A}/\hbar\right|^2}{4\pi}$ (2D) $= \frac{\left|\vec{k} - q\vec{A}/\hbar\right|^3}{6\pi^2}$ (3D) . (2) $\omega_c = \frac{qvB}{\hbar\left|\vec{k} - q\vec{A}/\hbar\right|}$

(3) Density of states per unit area($\frac{D(E)}{WL}$) is given by $\frac{dn}{dE}$, see Section 6.2, QTAT (Quantum Transport: Atom to Transistor, Cambridge 2005), page 138.

(b) Show that $\sigma_{zz} = q^2 n\tau / m$ if m is defined as $\frac{\hbar k}{v}$ where k and v denote the magnitude of the corresponding vectors $\vec{k}$ and $\vec{v}$.