## ECE 659 Spring '09

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

## Weeks 1-3: Semiclassical Transport, Summary

Fermi function: $\quad f(E)=1 /(1+\exp ((E-\mu) / k T))$
Current $\quad I=\frac{q}{h} \int d E \pi \gamma D(E)\left(f_{1}(E)-f_{2}(E)\right)$
Ballistic / diffusive transport: $\gamma=\hbar v_{z} / L, \quad I=q \int d E \underbrace{\frac{D v_{z}}{2 L}}_{\equiv M(E) / h}\left(f^{+}(E)-f^{-}(E)\right)$

$$
=q \int d E \frac{D(E)}{2 L} \frac{v_{z} \lambda}{\lambda+L}\left(f_{1}(E)-f_{2}(E)\right), \quad \lambda=2 v_{z} \tau
$$

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

$$
\begin{aligned}
& \frac{d f^{+}}{d z}=\frac{d f^{-}}{d z}=-\frac{f^{+}-f^{-}}{\lambda}, \quad \lambda \equiv 2 v_{z} \tau \\
& f^{+}(z, E)-f^{-}(z, E)=\frac{\lambda}{\lambda+L}\left(f_{1}(E)-f_{2}(E)\right)
\end{aligned}
$$

Linear Response: $\quad I \approx \int d E\left(-\frac{\partial f}{\partial E}\right) \tilde{I}(E), \quad \Delta \mu \ll k T$

$$
\begin{aligned}
\tilde{I} \approx q \frac{D(E)}{2 L} v_{z}\left(\mu^{+}-\mu^{-}\right) & =q^{2} \frac{D(E)}{2 L} \frac{v_{z} \lambda}{\lambda+L}\left(\frac{\mu_{1}-\mu_{2}}{q}\right) \\
& =\underbrace{q^{2} \frac{D(E)}{W L} \frac{v^{2} \tau}{d}}_{\equiv \tilde{\sigma}(E)} \frac{W}{\lambda+L} V \text { (d=2 for 2D, 3 for 3D) }
\end{aligned}
$$

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


Hall voltage (in $x$-direction):

$$
\begin{gathered}
V_{H}=\frac{2 \omega_{c} W}{\pi v}\left(\frac{\mu^{+}-\mu^{-}}{q}\right) \rightarrow \tilde{I}=q^{2} \frac{D(E)}{W L} \frac{v^{2}}{d \omega_{c}} V_{H} \\
\left\{\begin{array}{l}
V \\
V_{H}
\end{array}\right\}=\frac{1}{\tilde{\sigma}}\left[\begin{array}{cc}
L / W & -\omega_{c} \tau \\
+\omega_{c} \tau & W / L
\end{array}\right]\left\{\begin{array}{l}
\tilde{I} \\
\tilde{I}_{H}
\end{array}\right\} \rightarrow\left\{\begin{array}{l}
\tilde{I} \\
\tilde{I}_{H}
\end{array}\right\} \approx \tilde{\sigma}\left[\begin{array}{cc}
W / L & +\omega_{c} \tau \\
-\omega_{c} \tau & L / W
\end{array}\right]\left\{\begin{array}{l}
V \\
V_{H}
\end{array}\right\} \\
\sigma_{z z}=\int d E\left(-\frac{\partial f}{\partial E}\right) \tilde{\sigma}(E), \quad \sigma_{z x} \approx \int d E\left(-\frac{\partial f}{\partial E}\right) \tilde{\sigma}(E) \omega_{c} \tau
\end{gathered}
$$

where $\tilde{\sigma}(E) \equiv q^{2} \frac{D(E)}{W L} \frac{v^{2} \tau}{d}$, cf. Eqs.(4.33) and (4.60) in
Lundstrom, Fundamentals of Carrier Transport, Cambridge (2000).

## Scattering Theory of Transport:

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

## Two-probe conductance,

$$
\begin{align*}
Y & =\left(q^{2} / h\right)[I-S][M]=\left(q^{2} / h\right)[M-\bar{S}]  \tag{Total}\\
Y & =\left(q^{2} / h\right) 2[I-S][I+S]^{-1}[M] \\
& =\left(q^{2} / h\right) 2[M-\bar{S}][M+\bar{S}]^{-1}[M]
\end{align*}
$$

(Channel only)

Four-probe conductance, $\quad S=\left[\begin{array}{cc}A & C \\ D & B\end{array}\right], \quad P=[A]+[C][I-B]^{-1}[D]$

$$
\begin{aligned}
& \bar{A} \equiv[A]\left[M_{A}\right], \quad \bar{B} \equiv[B]\left[M_{B}\right], \quad \bar{C} \equiv[C]\left[M_{B}\right], \quad \bar{D} \equiv[D]\left[M_{A}\right] \\
& \quad[\bar{P}] \equiv[P]\left[M_{A}\right]=[\bar{A}]+[\bar{C}]\left[M_{B}-\bar{B}\right]^{-1}[\bar{D}] \\
& \rightarrow Y_{2 p t}=\frac{i_{A}}{V_{A}}=\left(q^{2} / h\right)[I-P]\left[M_{A}\right]=\left(q^{2} / h\right)\left[M_{A}-\bar{P}\right] \\
& \rightarrow Y_{4 p t}=\frac{i_{A}}{V_{B}}=\left(q^{2} / h\right)[I-P] D^{-1}[I-B]\left[M_{B}\right] \\
& \\
& =\left(q^{2} / h\right)\left[M_{A}-\bar{P}\right] \bar{D}^{-1}\left[M_{B}-\bar{B}\right]
\end{aligned}
$$

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

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

Assuming, $E(\vec{x}, \vec{k})=\sum_{j} \frac{\left(\hbar k_{j}-q A_{j}(\vec{x})\right)^{2}}{2 m}+U(\vec{x})$

$$
\begin{aligned}
& \rightarrow v_{i} \equiv \frac{d x_{i}}{d t}=\frac{\hbar k_{i}-q A_{i}(\vec{x})}{m}, \quad \hbar \frac{d k_{i}}{d t}=-\frac{\partial U}{\partial x_{i}}+q \sum_{j} v_{j} \frac{\partial A_{j}}{\partial x_{i}} \\
& \frac{d}{d t}\left(\hbar k_{i}-q A_{i}(\vec{x})\right)=-\frac{\partial U}{\partial x_{i}}+q \sum_{j} v_{j}\left(\frac{\partial A_{j}}{\partial x_{i}}-\frac{\partial A_{i}}{\partial x_{j}}\right)=-\frac{\partial U}{\partial x_{i}}+q \sum_{j, n} v_{j} \varepsilon_{i j n}(\vec{\nabla} \times \vec{A})_{n} \\
& \rightarrow \vec{v}=\frac{\hbar \vec{k}-q \vec{A}(\vec{x})}{m}, \\
& \frac{d(\hbar \vec{k}-q \vec{A})}{d t}=q(\vec{F}+\vec{v} \times \vec{B}) \quad \text { where } \quad q \vec{F}=-\vec{\nabla} U \text { and } \vec{B}=\vec{\nabla} \times \vec{A}
\end{aligned}
$$

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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 $\frac{R_{4 p t}}{R_{2 p t}}=\frac{\mu_{3}-\mu_{4}}{\mu_{1}-\mu_{2}}$, (a) if the voltage probes float to the local average electrochemical potential, $\left(\mu^{+}+\mu^{-}\right) / 2$ ? (b) if probe 3 floats to $\mu^{-}$and probe 4 floats to $\mu^{+}$?

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

$$
\bar{S}=[S][M]=\left[\begin{array}{cccc}
r_{1} & t^{\prime} & a^{\prime} & c^{\prime} \\
t & r_{2} & b^{\prime} & d^{\prime} \\
a & b & r_{3} & 0 \\
c & d & 0 & r_{4}
\end{array}\right] \text { with the reflection coefficients } r_{1,2,3,4} \text { determined by }
$$

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. $\left\{\begin{aligned} a^{\prime}+b^{\prime} & =a+b \\ c^{\prime}+d^{\prime} & =c+d \\ a^{\prime}+c^{\prime}+t^{\prime} & =a+c+t \\ b^{\prime}+d^{\prime}+t & =b+d+t^{\prime}\end{aligned}\right.$
(a) Show that $1 / R_{2 p t}=t+\frac{a b^{\prime}}{a+b}+\frac{c d^{\prime}}{c+d}=t^{\prime}+\frac{a^{\prime} b}{a+b}+\frac{c^{\prime} d}{c+d}$

$$
R_{4 p t}=\quad R_{2 p t} \frac{a d-b c}{(a+b)(c+d)}
$$

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 $a=a^{\prime}=\frac{K \lambda}{\lambda+L_{1}}, b=b^{\prime}=\frac{K \lambda}{\lambda+L_{2}+L_{3}}, c=c^{\prime}=\frac{K \lambda}{\lambda+L_{1}+L_{2}}, d=d^{\prime}=\frac{K \lambda}{\lambda+L_{3}}$ and $t=t^{\prime}=\frac{\lambda}{\lambda+L}$ with $L=L_{1}+L_{2}+L_{3}$, show that $R_{2 p t} \approx L / \lambda$ and $R_{4 p t} \approx L_{2} / \lambda$ for small K.
(c) Plot numerically the two-terminal resistance $R_{2 p t}$ and the four-terminal resistance $R_{4 p t}$ versus $\log (\mathrm{K})$, assuming $L_{1}=100 \lambda, L_{2}=20 \lambda, L_{3}=200 \lambda$, for $1 \mathrm{e}-3<\mathrm{K}<1$.
3. Consider a 2-D material like graphene having

$$
E(\vec{x}, \vec{k})=v_{f}|\hbar \vec{k}-q \vec{A}|+U(\vec{x})
$$

Starting from the equations for semiclassical dynamics $\frac{d \vec{x}}{d t}=\frac{1}{\hbar} \vec{\nabla}_{k} E, \frac{d \vec{k}}{d t}=-\frac{1}{\hbar} \vec{\nabla} E$
obtain expressions for $\frac{d \vec{x}}{d t}$ and $\frac{d(\hbar \vec{k}-q \vec{A})}{d t}$ and show that they agree with the usual result for parabolic bands with $E(\vec{x}, \vec{k})=(\hbar \vec{k}-q \vec{A})^{2} / 2 m+U(\vec{x})$
if we define mass as $m=|\hbar \vec{k}-q \vec{A}| /|\vec{v}|=(E-U) / v_{f}{ }^{2}$.
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 $\left(-\frac{\partial f}{\partial E}\right) \simeq \delta\left(E-E_{f}\right)$ and all conductivities are determined by a single energy $E=E_{f}$ :

$$
\begin{aligned}
\sigma_{z z}(E) & =q^{2} \frac{D(E)}{W L} \frac{v^{2} \tau}{d} \\
\rho_{z x}(E) & =\frac{\omega_{c} \tau}{\sigma_{z z}(E)}
\end{aligned}
$$

(a) Show that $\rho_{z x}=\frac{B}{q n}$ in both 2D and 3D.

$$
\begin{aligned}
n & =\frac{|\vec{k}-q \vec{A} / \hbar|^{2}}{4 \pi} \text { (2D) } \\
& =\frac{|\vec{k}-q \vec{A} / \hbar|^{3}}{6 \pi^{2}} \text { (3D) }
\end{aligned}
$$

(3) Density of states per unit area $\left(\frac{D(E)}{W L}\right)$ is given by $\frac{d n}{d E}$, see Section 6.2, QTAT
(Quantum Transport: Atom to Transistor, Cambridge 2005), page 138.
(b) Show that $\sigma_{z z}=q^{2} n \tau / m$ if $m$ is defined as $\frac{\hbar k}{v}$ where $k$ and $v$ denote the magnitude of the corresponding vectors $\vec{k}$ and $\vec{v}$.

