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/

Final exam: Thursday, 5/7, 7PM - 9PM, Lawson, B155

Cumulative, Closed book, notes (4 pages) will be provided

General References

1. Chapter 1, 4, 7.1, 8-11: Quantum Transport: Atom to Transistor
2. Lectures 1-5A, 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 final exam, one from each of the topics we have covered: Semiclassical transport, quantum transport, spin transport, energy transport and correlated transport. The homework problems (without the MATLAB implementation) are a good guide. The last practice exam is also a good guide regarding the first two topics. In addition the following problems are intended to be a guide to the last three topics.

Problem 1: A two-component spinor $\{\psi\}$ evolves in time according to the equation $i\hbar \frac{d}{dt}\{\psi\} = \mu_B[\vec{\sigma}.\vec{B}]\{\psi\}$, where $\vec{\sigma}$ represents the Pauli spin matrices. Show that the spin $\vec{S} \equiv \psi^+ \vec{\sigma} \psi$ evolves according to $\frac{d}{dt}\vec{S} = \frac{2\mu_B}{\hbar}\vec{B} x \vec{S}$. ***Useful result:*** $\left(\vec{a} x \vec{b}\right)_m = \varepsilon_{mnp} a_n b_p$

Problem 2: Consider a channel with two spin levels, described by a (2x2) Hamiltonian $[H] = \varepsilon_0 I + \varepsilon \sigma_z$, connected to two anti-parallel contacts 1and 2, one communicating exclusively with +x spins and the other with -x spins. (a) Write down the self-energy matrices Σ_1 and Σ_2. (b) Calculate the spectral function [A]. A small bias is applied so that over a small energy range around E = 0 where we can assume f_1=1 and f_2=0. Find (c) the correlation function G^n and (d) the number of electrons N and the spin $\vec{S}$ in the channel.

Problem 3: Consider a 2-D conductor in the x-y plane described by the Hamiltonian

$$H = \frac{p^2}{2m} + C\vec{\sigma}.\left(\vec{\mathrm{E}} x \vec{p}\right)$$

where m is the effective mass, C is a real constant and $\vec{\mathrm{p}} \equiv -i\hbar\vec{\nabla}$. There is a strong electric field perpendicular to the plane of the conductor : $\vec{\mathrm{E}} = \mathrm{E}_0 \hat{z}$. Assume a plane wave solution of the form $\exp[i(\vec{k}.\vec{r} - Et/\hbar)] \begin{pmatrix} \psi \\ \overline{\psi} \end{pmatrix}$, where $\vec{k}$ lies in the x-y plane and obtain the dispersion relation $\mathrm{E}(\vec{\mathrm{k}})$.

Problem 4: Starting from $\left[\Sigma_s^{in}(E)\right] = D(+\varepsilon)\left[G^n(E-\varepsilon)\right]$

and $\left[\Gamma_s(E)\right] = D(+\varepsilon)\left[G^n(E-\varepsilon)\right] + D(+\varepsilon)\left[G^p(E+\varepsilon)\right]$ show that

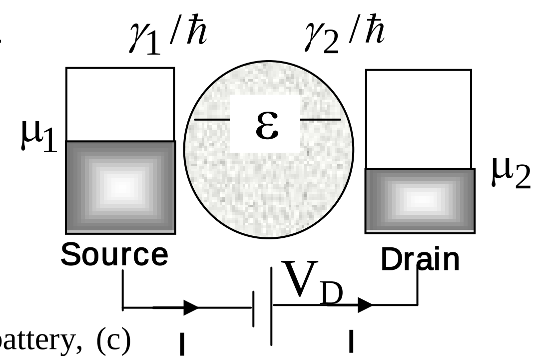
(a) the integrated scattering current is zero, though it may not be zero at each energy E:

$$\int dE\; I_i(E) = \frac{q}{h}\int dE\; Trace[\Sigma_s^{in}A - \Gamma_s G^n] \;= 0$$

(b) the scattering current is zero at each energy if both the electrons and the scatterers are at equilibrium at the same temperature T.

Problem 5: Consider a device having one energy level ε with equal escape rates $\gamma_1/\hbar = \gamma_2/\hbar = 10^{12}$ /sec . (small enough that the broadening can be neglected) with an applied voltage $V_D = (\mu_1 - \mu_2)/q$ such that

$\varepsilon - \mu_1 = k_B T$ and $\varepsilon - \mu_2 = 2k_B T$



Calculate the (a) current, (b) power delivered by the battery, (c) power dissipated in (or absorbed from) contact 1 and (d) power dissipated in (or absorbed from) contact 2. Assume $k_B T$ = 0.025 eV.

Problem 6: A channel has two energy levels ε_1 and ε_2 corresponding to four levels 00, 01, 10 and 11 in the multi-electron picture. Apply the law of equilibrium in the multi-electron picture to obtain the equilibrium occupation probabilities assuming zero interaction energy (U_0 = 0) for the four levels and show that

$$P_{00} = (1 - f_1)(1 - f_2) \;\;,\; P_{01} = (1 - f_1)\, f_2,\;\; P_{10} = f_1(1 - f_2) \text{ and } P_{11} = f_1 f_2$$

where f_1 and f_2 are the equilibrium Fermi functions corresponding to the two energy levels.

Problem 7: A channel has a very large number N of degenerate states all having the same energy ε in equilibrium with an electrochemical potential µ and temperature T. Starting from the general law of equilibrium $P_n = (1/Z)\, e^{-(E_n - n\mu)/k_B T}$, show that the fraction of occupied states can be written as $f \equiv \dfrac{n}{N} = \dfrac{1}{\exp\left(\dfrac{\varepsilon + \alpha - \mu}{k_B T}\right) + 1}$ if the interaction energy U(n) can be approximated as $U(n) \cong U_0 + \alpha n$. ***Useful result:*** $\sum_n {}^N C_n\, x^n = (1+x)^N$, $\sum_n {}^N C_n\, n\, x^n = Nx(1+x)^{N-1}$

Problem 8: Consider two coupled quantum dots each with two spin-degenerate levels, such that the one-electron Hamiltonian,

$$h = \begin{array}{c} \begin{array}{cccc} a & b & \bar{a} & \bar{b} \end{array} \\ \begin{bmatrix} \varepsilon & t & 0 & 0 \\ t & \varepsilon & 0 & 0 \\ 0 & 0 & \varepsilon & t \\ 0 & 0 & t & \varepsilon \end{bmatrix} \end{array}$$

having an intra-dot interaction energy U and zero inter-dot interaction energy.

At what values of µ does the total number of electrons change from N = 0 to 1 to 2 to 3 and finally to 4?

Useful result: Eigenvalues of $\begin{bmatrix} a & 0 & t & t \\ 0 & a & t & t \\ t & t & b & 0 \\ t & t & 0 & b \end{bmatrix}$

are a, b and $\dfrac{(a+b) \pm \sqrt{(a-b)^2 + 16t^2}}{2}$