ECE 5390/MSE 5472, Fall Semester 2015
Quantum Transport in Electron Devices & Novel Materials

Debdeep Jena (djena@cornell.edu), Depts. of ECE and MSE, Cornell University

Assignment 3

Policy on assignments: Please turn them in by 5pm of the due date. The due date for this assignment is **Friday, Oct 9th, 2015**.

General notes: Present your solutions *neatly*. Do not turn in rough unreadable worksheets - learn to **take pride in your presentation**. Show the relevant steps, so that partial points can be awarded. $\boxed{\text{BOX}}$ your final answers. Draw figures wherever necessary. Please print out this question sheet and staple to the top of your homework. Write your name and email address on the cover. Some problems may lead to publishable results - be on the lookout!

Problem 3.1) Ballistic FET design for high-speed linear amplifiers

In class we discussed that for a Ballistic FET with a 2D electron gas channel, a parabolic bandstructure $E(k_x, k_y) = \frac{\hbar^2}{2m^\star}(k_x^2 + k_y^2)$ leads to a current $\frac{I_d}{W} \propto (V_{gs} - V_T)^{\frac{3}{2}}$, leading to a gain or transconductance $g_m = \frac{\partial I_d}{\partial V_{gs}} \propto (V_{gs} - V_T)^{\frac{1}{2}}$.

(a) Show why if the gate is driven by a monochromatic input signal $V_{gs} = V_{gs}^{dc} + v_\omega e^{i\omega t}$, the output ac current has many frequencies, not just the frequency of the input signal.

(b) Assume $v_\omega << V_{gs}^{dc}$. Can you design a bandstructure that will remove these higher harmonics?

Problem 3.2) Using the Landauer formula to explain the broadening of experimental conductance quantization steps

We derived the expression for current :

$$\mathbf{J} = \frac{q g_s g_v}{L^d} \sum_{\mathbf{k}} \mathbf{v}_g(\mathbf{k}) T(\mathbf{k}) \Big[f_L(\mathbf{k}) - f_R(\mathbf{k}) \Big], \tag{1}$$

where $T(\mathbf{k})$ is the transmission probability for mode[1] $|\mathbf{k}\rangle$. In the ballistic FET problem for example, we used the approximation $T(\mathbf{k}) = 0$ for $E(\mathbf{k}) < W_0$ and $T(\mathbf{k}) = 1$ for $E(\mathbf{k}) > W_0$, where W_0 is the conduction band-edge barrier height controlled by the gate. In assignment problem 2.2, you found the current through a *rectangular* barrier, for which you had derived an *exact* transmission $T(\mathbf{k})$ in assignment problem 1.3. Equation 1 is the Landauer formula in disguise; in this problem, we gain a deeper insight into the Landauer formula, and use it to explain an experimental feature of quantized conductance: why the conductance quantization steps are not very sharp. This has to do with tunneling, when $0 < T(\mathbf{k}) < 1$.

[1] The more general form for the Landauer formula reads $I = \frac{q g_s g_v}{2\pi} \int_{-\infty}^{+\infty} dE \cdot \mathrm{Tr}[\hat{t}^\dagger \hat{t}] \cdot [f_L(E) - f_R(E)]$, where $\mathrm{Tr}[\hat{t}^\dagger \hat{t}]$ is the *trace* of $\hat{t}^\dagger \hat{t}$, where $\hat{t}$ is the transmission matrix of the amplitudes of individual modes. For a *single* mode, it is the plain vanilla complex number amplitude t whose square $t^\dagger t = |t|^2 = 1 - |r|^2$ is the transmission probability. The transmission matrix $\hat{t}$ retains the interference terms in the amplitudes, which are lost in summing the squares $|t|^2$.

(a) Consider two contacts with electrochemical potentials μ_L and μ_R separated by an *arbitrary* shaped 1D potential barrier $W(x)$. For a mode of energy $E(k_x)$ that has a group velocity $v(k_x)$, consider the components of the current between the left electrode and the barrier. The carriers there could have come from *three* sources: (1) directly from the left contact, (2) reflected from the barrier with amplitude r_{k_x}, and (c) transmitted through the barrier with amplitude t_{k_x}. Show that if the transport is elastic (no energy loss), the current carried by the mode is

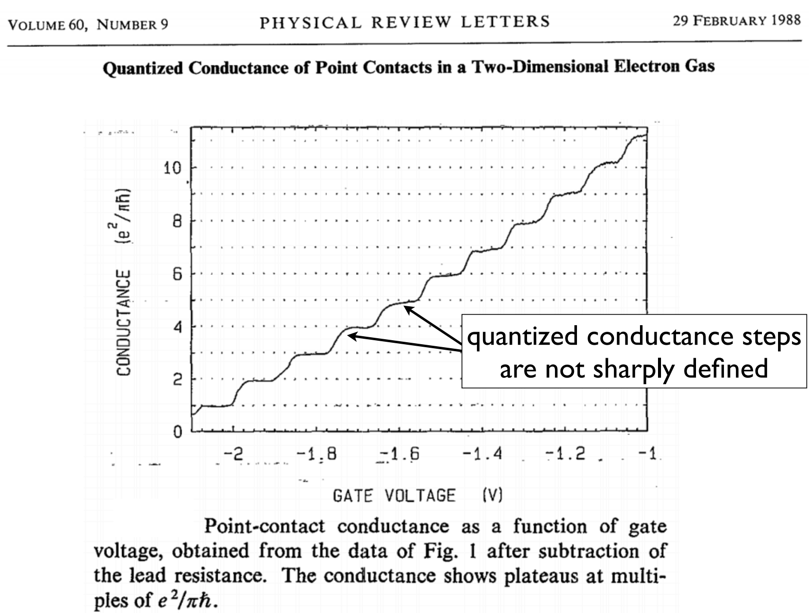
$$I_{k_x} = \frac{q g_s g_v}{L} v(k_x) \Big[f_L(k_x) - |r_{k_x}|^2 f_L(k_x) - |t_{k_x}|^2 f_R(k_x) \Big], \tag{2}$$

where f_L and f_R are the Fermi functions of the contacts. Show that Eq. 2 directly leads to Eq. 1.

(b) Show that the current for a multi-channel (multiple subband) conductor is

$$I = G_0 \sum_n \frac{1}{q} \int_{-\infty}^{+\infty} dE \cdot |t_n(E)|^2 \big[f_L(E) - f_R(E) \big], \tag{3}$$

where $G_0 = \frac{g_s g_v q^2}{h}$ is the conductance quantum. Show that for $T \to 0$ K, if $|t_n(E)|^2 = 1$, then the conductance $G = I/V$ is $\boxed{G = G_0 M}$, where M is the number of channels whose energies lie between $\mu_L < E < \mu_R$. This is the celebrated Landauer formula.


VOLUME 60, NUMBER 9 PHYSICAL REVIEW LETTERS 29 FEBRUARY 1988

Quantized Conductance of Point Contacts in a Two-Dimensional Electron Gas

Point-contact conductance as a function of gate voltage, obtained from the data of Fig. 1 after subtraction of the lead resistance. The conductance shows plateaus at multiples of $e^2/\pi\hbar$.

Figure 1: Broadening of the quantized conductance steps.

(c) Now consider the measured conductance in Figure 1. This conductance is measured using a split-gate constriction that changes the effective number of modes passing through the constriction. Clearly the conductance steps are not sharply defined, and there is also broadening between steps. Can you explain this feature by identifying the reason, and outlining a method you may go about *quantitatively* calculating it?

Problem 3.3) WKB: Tunneling, and Flash Memory

Figure 2 shows a 1-dimensional potential for an electron, which is in the state with energy E_0 at $t = 0$. Since there is a lower potential for $x > L_w + L_b$, the state $|E_0\rangle$ is a *quasi-bound* state. The electron is destined to leak out.

(a) Using WKB tunneling probability, and combining semi-classical arguments, find an analytical formula that estimates the time it takes for the electron to leak out. Find a value of this lifetime for $L_b \sim 3$ nm, $L_w \sim 2$ nm, $V_0 \sim 1$ eV, $E_0 \sim 2$ eV, and $E_b \sim 5$ eV. How many years does it take?

(b) This feature is at the heart of *flash memory*, which you use in computers and cell phones. Find an analytical expression that describes how the lifetime changes if a voltage V_a is applied across the insulator. Estimate the new lifetime for $V_a \sim 2.8$ V. This is the *readout* of the memory.

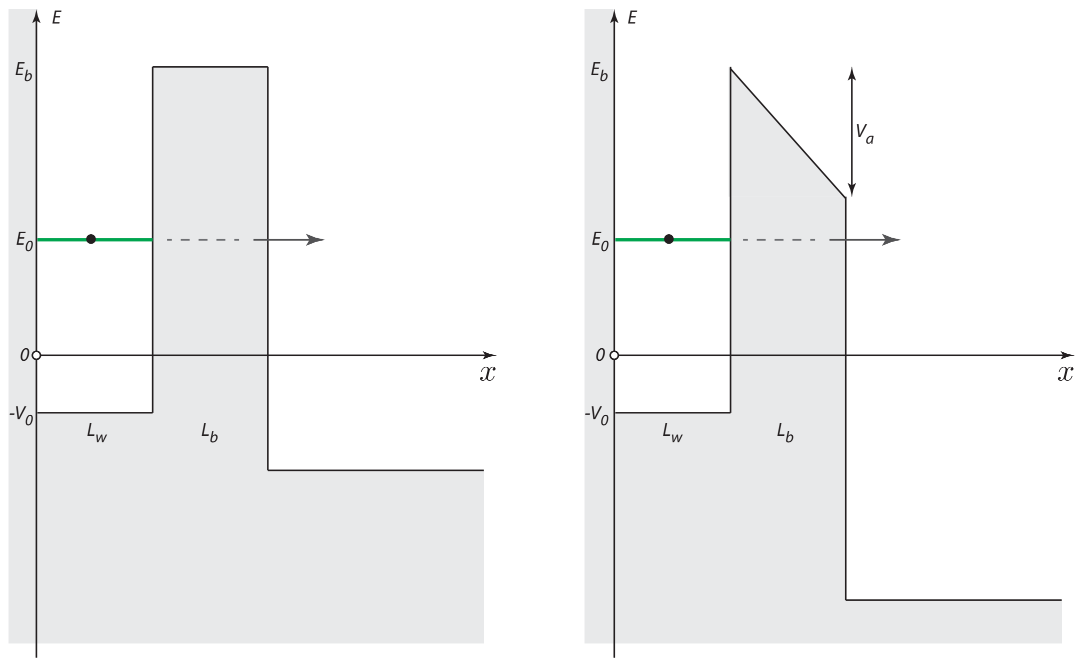


Figure 2: Escape and field-emission by tunneling.

Problem 3.4) Green's Functions, Self-Energy, Transport Through Dots

We re-cast the problem of electron current in terms of the non-equilibrium Green's functions (NEGF) formalism. The basic strategy was to convert a *closed* quantum system with Schrodinger equation $i\hbar\frac{d\psi}{dt} = H\psi$ to an *open* quantum system by the introduction of a self-energy and source term: $i\hbar\frac{d\psi}{dt} = H\psi + \Sigma\psi + s$. We defined the Green's function as $G(E) = (EI - H - \Sigma)^{-1}$. By defining the anti-Hermitian parts of the self-energy matrices for reservoir m as $\Gamma_m = i(\Sigma_m - \Sigma_m^\dagger)$, and the source-influx as $\Sigma_{in} = \Gamma_1 f_1 + \Gamma_2 f_2$, we identified the correlation function as $G_n(E) = G\Sigma_{in}G^\dagger$, and the spectral function as $A(E) = i(G - G^\dagger)$. The density of states of the system was found to be $D(E) = \text{Trace}[A(E)]/2\pi$. The transmission was found to be $T_{12}(E) = \text{Trace}[\Gamma_1 G \Gamma_2 G^\dagger]$, the current spectrum $\tilde{I}_1(E) = \frac{q}{h}T_{12}(E)[f_1(E) - f_2(E)]$, and the net current was $I_1 = \int_{-\infty}^{+\infty} dE\tilde{I}_1(E)$. Neglect spin throughout this problem.
Consider the problem of transport through a quantum dot sitting in a wide-bandgap insulator between two metal electrodes. A single energy eigenvalue E_0 of the *isolated* dot falls between the metal Fermi levels of interest. Assume that the coupling to the left and right electrodes measured by the self-energy term is identical, both being $\Sigma = \epsilon_0 + i\eta$.

(a) Calculate the density of states of this system, and show its dependence on η. Prove that if we started with one energy state, the integral of the broadened DOS is still unity. Explain.

(b) Calculate the current through the dot as a function of the voltage at any temperature.

(c) Make a plot of the density of states and the I-V curves at $T = 300$ K and $T = 4$ K for $E_0 = 1$ eV, $\epsilon_0 = 0.01$ eV, and $\eta = 0.1$ eV.

(d) Show that the conductance can not exceed the quantum of conductance $G_0 = \frac{I}{V} \leq \frac{e^2}{h}$.

Problem 3.5) Conductivity by Non-Equilibrium Green's Functions (NEGF)

In class we discussed a 2-site 1D chain to illustrate the NEGF method for evaluating quantum transport. In Problem 3.4, you did the 1-site problem, for which analytical results are available. Here, you will set up a 4-site transport problem. Assume the uncoupled on-site energies to be $E_0 = 4$ eV, the hopping energy $t = 1$ eV, and the 'contacts' to be identical to the inter-site hopping terms. Plot i) the system DOS, ii) the transmission $T(E)$, and iii) the I-V curves at $T = 300$K and $T = 4$K.