

ECE 587/687 — FUNDAMENTALS OF NANOELECTRONICS

UNIVERSITY OF VIRGINIA

Spring 2009

Take-Home Final, Due Wednesday May 6th

(print name above)

Please show all your work, and give clear answers. Attach numerical code if used. Usual disciplinary issues apply – no unauthorized assistance of any sort is allowed. You can consult your textbook, slides, HW solutions and class notes. You are allowed to look up the internet just to extract the parameter values for Problem 3.

Answer all 4 problems

Problem 1(25%): _____ Problem 2(25%): _____

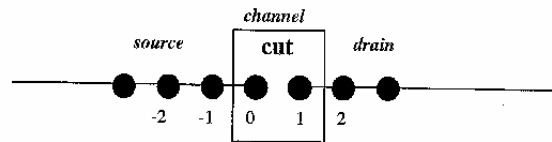
Problem 3(25%): _____ Problem 4(25%): _____

TOTAL(100%): _____

On my honor as a student, I have neither given nor received unauthorized assistance on this exam.

(sign name above)

Problem 1 (Current conduction) [25 points].



Consider a wire with a cut. In a basis set of one orbital per wire atom, it is easy to write down the Hamiltonian of the two atom device, boxed above, as $H = \begin{bmatrix} 2t & 0 \\ 0 & 2t \end{bmatrix}$.

1. What are the self-energies $\Sigma_{1,2}$ and the broadenings $\Gamma_{1,2}$ due to the two 1-D contacts shown? (Remember each must be a 2x2 matrix). Keep your answers in terms of E , t and ka [2 x 5 = 10]

2. Calculate the Green's function G (do not just write down the formula – evaluate the inverse matrix). [5]

3. Calculate the transmission $\bar{T}(E) = \text{trace}[\Gamma_1 G \Gamma_2 G^\dagger]$. Does this make sense? [8+2]

Problem 2 (Heat flow) [25 points]

1. In an earlier exam, you calculated the charge current and determined the electronic conductance quantum. Let us now try to find the thermal conductance quantum with an analogous process. We impose a *temperature difference* instead of a *voltage difference* between two contacts so that $\mu_1 = \mu_2 = \mu$, but $T_1 = T_2 + \Delta T$. The thermal current is given by

$$I_Q = \frac{2}{h} \int dE \bar{T}(E)(E - \mu) \left[f_1(E) - f_2(E) \right] \quad (1)$$

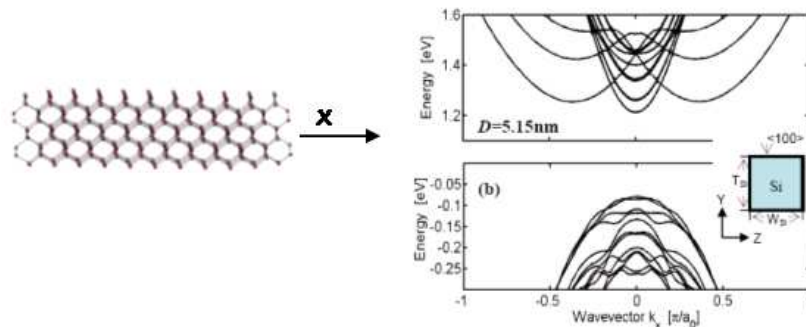
where the energy (or thermal ‘charge’) injected by each contact is proportional to $E - \mu$, while the Fermi function difference arises from the temperature difference.

Assuming a *ballistic* channel, let’s try to calculate this thermal current. Taylor expand the difference $f_1(E) - f_2(E) \approx \Delta T \cdot \partial f(E)/\partial T$. Given that $f(E) = 1/[1 + e^x]$ where $x = (E - \mu)/k_B T$, simplify the leading term (for a given T) as a compact function of x . *Keep the chain rule in mind.* [15]

2. Substituting this expression into the thermal current integral, changing variables to $x = (E - \mu)/k_B T$, and using one of the integrals provided at the back of the exam, write down the thermal conductance quantum $\kappa = I_Q/\Delta T$. It should be a compact ratio of a few terms only. [6]

3. Substituting the values $k_B = 1.38 \times 10^{-23} J/K$ and $h = 6.6 \times 10^{-34} Js$, find the value of κ in units of watts/kelvin (keeping in mind that 1 watt = 1J/s) [4].

Problem 3 (Bandstructure of a silicon nanowire) [25] The figure below shows the E-k for a silicon nanowire, oriented along the x-axis (k is a 1D vector since we have a 1D problem here). Our aim is to try to understand the *broad* features of this E-k near the conduction band (ie, an n-type nanowire). In other words, we will focus on some of the semi-quantitative aspects at the conduction band bottom, such as the locations of the minima, band offsets, masses etc and see if our bandstructure allows us to understand these.



Let us start with the E-k for a bulk silicon wire that we worked out for one of our HWs. Near the conduction band minimum (located at 0.815 per-cent of the Brillouin zone along the $\Gamma - X$ direction), one can fit a parabola to get the effective masses around them. There are six equivalent axes corresponding to the $\Gamma - X$ direction, namely, the $\pm k_x$, $\pm k_y$ and $\pm k_z$ axes. This means that the six E-k dispersions near these band minima can be written as $E_{1,2} = \hbar^2(k_x \pm k_0)^2/2m_l + \hbar^2(k_y^2 + k_z^2)/2m_t$ and cyclic permutations among $\{k_x, k_y, k_z\}$. For instance, the first band E_1 is centered around $k_x = k_0$, $k_y = 0$ and $k_z = 0$.

Let us now carve out a nanowire out of this bulk silicon template, by imposing box boundary conditions in the y-z directions corresponding to a width $W = 5.15\text{nm} = 51.5\text{\AA}$ in each direction. *To zeroth order, this simply quantizes the k_y and k_z values in terms of W and leaves k_x unchanged, so we can replot it vs k_x and get the 1-D nanowire band-diagram above.*

The only catch is the anisotropy ($m_l \neq m_t$), which means that at some of the six minima, k_x is the longitudinal coordinate with mass m_l , while at the others, it is the transverse coordinate with mass m_t . *This alone accounts for the complexity of the band-diagram above, as we shall see!*

1. By consulting the internet or your text book, list the values of (i) a (the *lattice constant* of Si in Angstroms – NOT the Si-Si bondlength), (ii) k_0 as a fraction of $(2\pi/a)$, and the (iii) longitudinal and (iv) transverse masses m_l and m_t in terms of the free electron mass m_0 , for silicon. [4]

2. (a) Show that four of the six equivalent $E - k$ bands, upon quantizing the k_y and k_z sets, are responsible for creating the 1D subbands at $k = 0$ in the above figure. Which four are they? (b) Why are they centered at $k = 0$? (Remember you are only looking at the conduction band, and that the actual answer has more features than you get from this effective mass analysis, since the atomistic simulations have many orbitals and higher bands) [3 + 3]

3. (a) Show that the remaining two (which two?) create 1D E-ks that are offset from $k = 0$ above. (b) What are these offset k values? (remember that the original k-values need to be folded into the new Brillouin zone, which runs from $-\pi/a$ to π/a . The way to fold them is to add a reciprocal lattice vector $\pm 2\pi/a$ so it is brought into this Brillouin zone. Check your calculated k value against the figure above) [2 + 4]

4. what are the effective masses of the two sets of bands you just calculated? (Once you start with the six bulk E-k bands, and eliminate the $k_{y,z}$ contributions which are quantized constants, the only variable is k_x that appears in the two sets of bands with its own effective mass. This would be a combination of m_l and m_t in each case) [2.5 + 2.5]

5. Given the masses m_l , m_t , and the width W (which creates different quantization conditions for the six original bands), find the vertical energy offset between the lowest conduction band (at $k=0$) and the other two next higher conduction bands. (This should agree with the plot) [4]

Problem 4 (Trap-channel interactions)[25]

Let us try to understand how a trap can block the current through a channel and create a drop in current. This is very relevant for present day devices. The trap is essentially a non-conducting level that communicates very weakly with the contacts (small γ s), so that once a charge is injected onto it, it stays there for a very long time. Filling the trap, however, pushes the conducting level (channel, with larger γ s) out of the conduction window through Coulomb repulsion, thus blocking the channel. *Our aim in this problem is to create a 'toy' numerical model for this trap-channel interaction.*

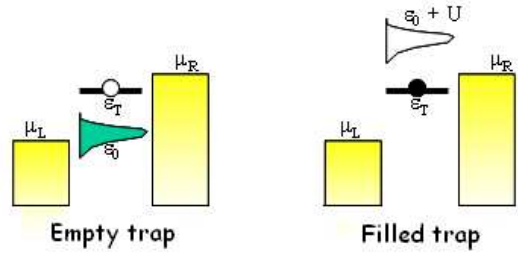
The energy diagram below shows a conducting channel centered around ϵ_0 , with equal couplings $\gamma_1 = \gamma_2$ to the contacts. The channel density of states is described by a broad Lorentzian $D_{ch}(E) = \frac{\gamma_1 + \gamma_2}{2\pi[(E - \epsilon_0)^2 + (\frac{\gamma_1 + \gamma_2}{2})^2]}$. The Fermi energy of the channel lies below

the level, so that the channel is initially empty. Let us start raising the drain electrochemical potential $\mu_2 = E_F + qV$ by putting a negative voltage on it relative to the source, which is held at $\mu_1 = E_F$. At some point, the channel is filled by the drain, and it starts conducting.

1. What is the expected maximum current through this level? Set up a toy model from chapter 1 to numerically compute the I-V through this system for a voltage range between zero and 0.6 V (*ignore Coulomb interactions and self-consistency*). Use the following parameters: $E_F = 0$, $\epsilon_0 = 0.2eV$, $\gamma_1 = \gamma_2 = 0.005eV$, $kT = 0.025eV$. Choose 101 voltage points in the voltage range between 0 and 0.6 V. For the energy integration needed to compute the current, choose 501 energy grid points between -4 to +4 eV. Does your maximum computed current agree with your analytical estimate? [3 + 5]

2. Let us now include a trap, which acts as another level with the same shape of the density of states as the channel, but different parameters ($\epsilon_1 = 0.4eV$, and weak couplings $\gamma_{1t} = \gamma_{2t} = 0.0005eV$ to the contacts. Once the drain voltage is high enough to fill the trap, you will get additional current from the trap. (We assume the levels themselves do not slip, in other words, no local Laplace or Poisson potential for either level).

What is the analytically expected *additional* current due to the trap (i.e., the current contribution from the trap alone?). Set up the numerical code to include this additional density of states (i.e., in your computed current, you now have a sum of two terms each proportional to the respective density of states and the γ combination). Does your computed current from the trap agree with your analytical estimate? [3 + 5]



3. Now, let's add the Coulomb repulsion from the trap onto the channel. The figure above shows the physics. Once the trap is filled, it does not increase the current substantially (since its γ s are low), but it can repel the channel out of the conduction window. To capture this, go back to the numerical code, and add a Coulomb potential $U_0 n_t$ to the channel energy ϵ_0 , where $U_0 = 1.25eV$ is the single-electron charging energy due to the trap, and n_t is the charge on the trap computed from our toy equations (recall the expression for the non-equilibrium charge N on a level, in terms of its integrated density of states, γ s, f s etc). In other words, the channel feels a Coulomb potential due to the trap (the trap level sees no Laplace or Coulomb potential and stays fixed).

Include this potential in your code (you compute n_t first and then use the corresponding potential as an added term to ϵ_0 to compute the shifted channel density of states, and then calculate current through both). What does the I-V show? Explain what is happening. What determines the current that is still left at high bias through this system. [7 + 2]

Equations that you may or may not need:

$$\begin{aligned}\int_0^\infty dx \frac{e^x}{(1+e^x)^2} &= 1/2 \\ \int_0^\infty dx \frac{xe^x}{(1+e^x)^2} &= \ln(2) \\ \int_0^\infty dx \frac{x^2 e^x}{(1+e^x)^2} &= \pi^2/6 \\ \int_{-\infty}^\infty \frac{dy}{y^2+x^2} &= \frac{\pi}{x}\end{aligned}\tag{2}$$

$$\begin{aligned}\begin{bmatrix} a & b \\ c & d \end{bmatrix}^{-1} &= \frac{1}{ad-bc} \begin{bmatrix} d & -b \\ -c & a \end{bmatrix} \\ \begin{bmatrix} a & b \\ c & d \end{bmatrix}^\dagger &= \begin{bmatrix} a^* & c^* \\ b^* & d^* \end{bmatrix}\end{aligned}\tag{3}$$