

6.701/6.719 Final Exam May 17th 2011

Name: _____

$$q = 1.6 \times 10^{-19} C$$

$$h = 6.63 \times 10^{-34} J \cdot s$$

$$k = 1.38 \times 10^{-23} \frac{J}{K}$$

$$m_e = 9.1 \times 10^{-31} kg$$

Question 1 This question relates to the molecule shown below.



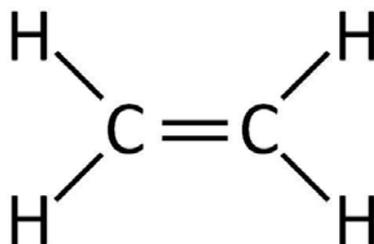
Answer the following under the assumptions:

- Born-Oppenheimer approximation
- Tight binding approximation
- $\alpha = \langle \varphi_i | T + V_i | \varphi_i \rangle$
- $\beta = \langle \varphi_i | V_i | \varphi_j \rangle$
- $\gamma = \langle \varphi_i | V_j | \varphi_i \rangle \approx 0$
- $S_{ij} = \langle \varphi_i | \varphi_j \rangle \approx 0$

a) Write the Hamiltonian matrix for this molecule in terms of α , β , and E.

b) Write the energy for this molecular orbital in terms of α and β .

c) Compare the density of states of the HOMO and LUMO of the previous molecule to the one below.



Question 2 The following question refers to ion channel mechanical switches at $T = 300\text{K}$.

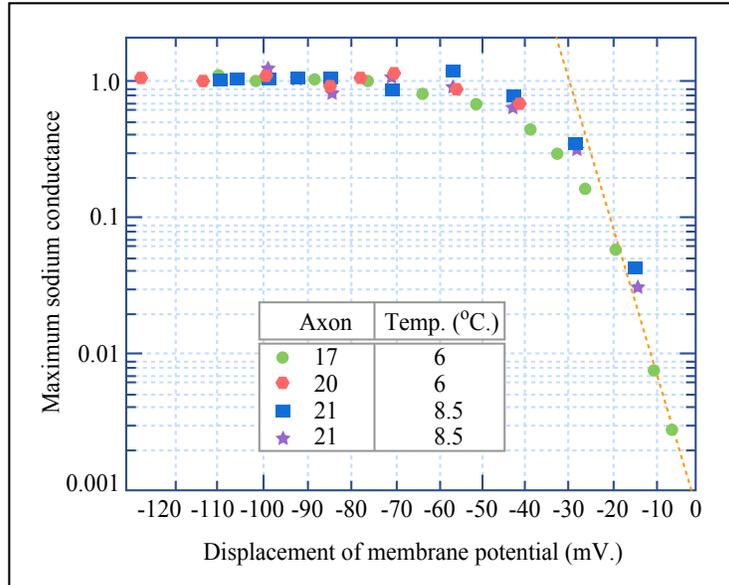


Image by MIT OpenCourseWare.

a) Assume that any given ion channel is either open with conductance $G = G_0$, or closed with conductance $G = 0$. Using Boltzmann statistics, write an expression for the conductance of a giant squid axon (with N ion channels in parallel) as a function of the applied membrane potential, V . Assume that the number of closed channels at $V = 0$ is N_0 .

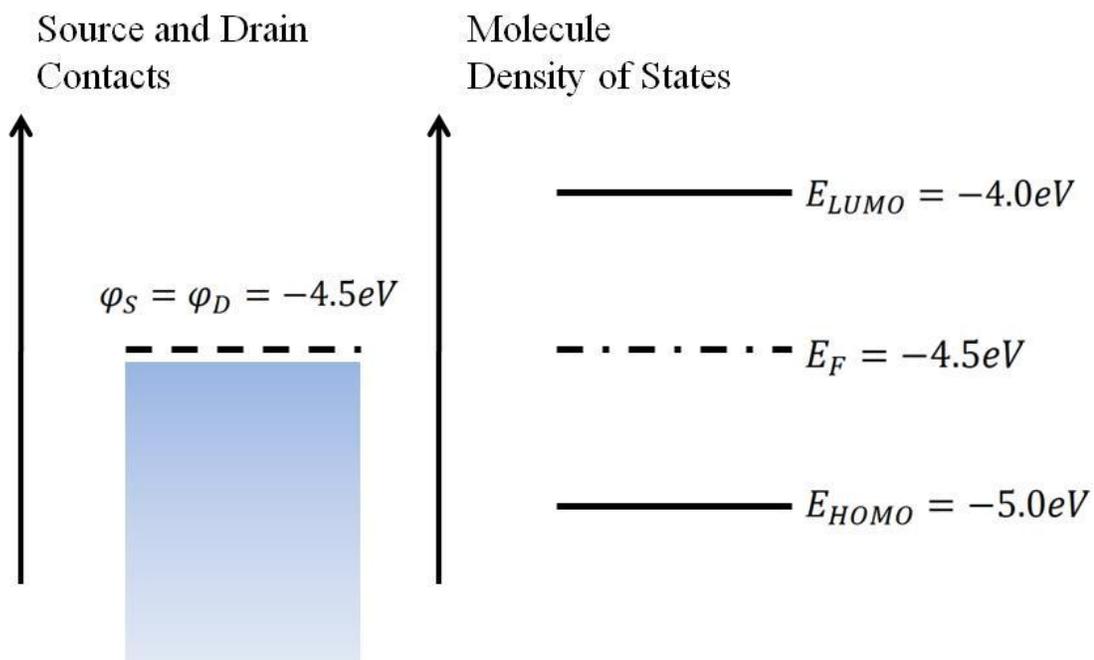
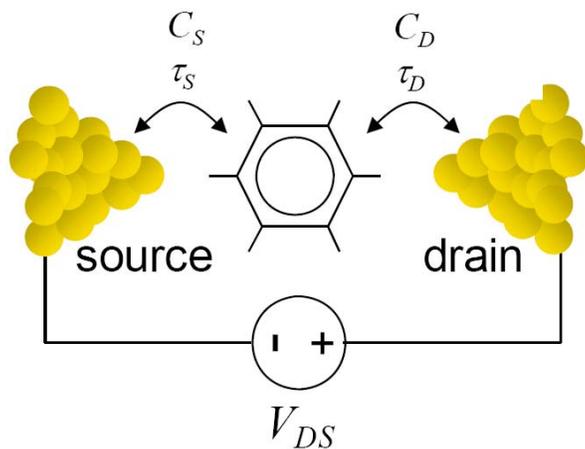
Hint: Given Boltzmann statistics, the relative populations N_1 and N_2 of two states separated by energy dU are $\frac{N_1}{N_2} = \exp\left(-\frac{dU}{kT}\right)$.

b) Where possible, evaluate your parameters for the data shown above.

c) Sketch a representative IV of a single ion channel.

Question 3 This problem refers to the 2 terminal molecular conductor below.

$T = 0\text{K}$



a) When $\tau_S = \tau_D = 1\mu s$, calculate the I_{DS} vs. V_{DS} characteristics for 0V to 3V and sketch it. Assume that the charging energy equals zero and $C_S = 2C_D$.

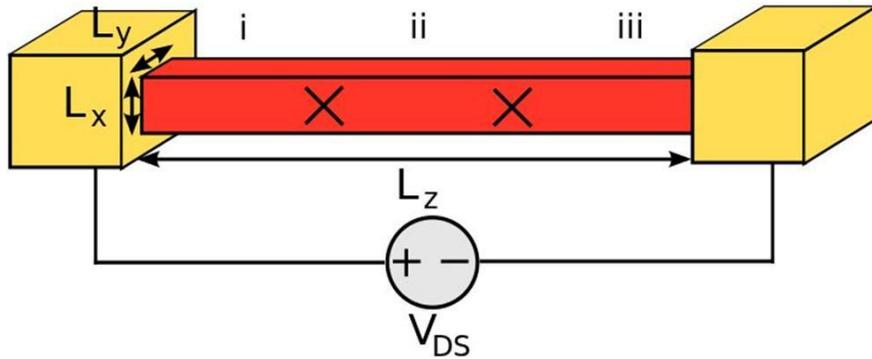
b) When $\tau_S = \tau_D = 1\mu s$, calculate the I_{DS} vs. V_{DS} characteristics for 0V to 3V and sketch it. Assume that the charging energy equals 1eV per electron and $C_S = 2C_D$.

c) In part a) and b), we have assumed that the HOMO of LUMO of the molecule are discrete energy levels. When $\tau_S = 10$ fs, $\tau_D = 5$ fs, calculate the actual molecular density of states versus energy. Determine the full width half maximum of HOMO and LUMO.

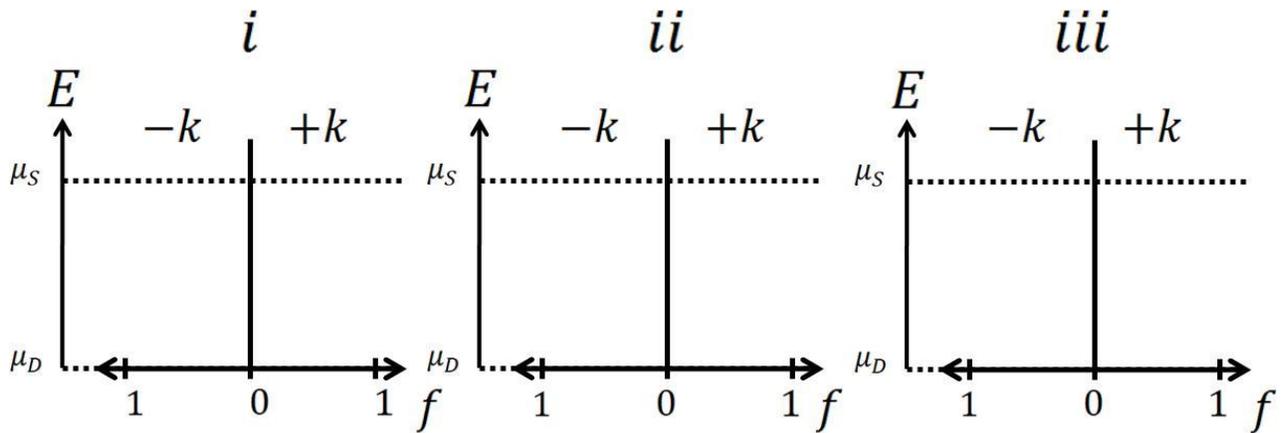
d) (6.719 only) Based on the actual density of states calculated in part c), find the number of electrons and the charging energy when the molecule is brought into contact with the metal electrode and reached equilibrium (no applied voltage). Also sketch the energy diagram at equilibrium. Assume that the charging energy per electron is 1eV and $\tau_S = 10$ fs, $\tau_D = 5$ fs.

Hint: You will need your calculator to solve this. You might use $\int \frac{1}{1+x^2} dx = \tan^{-1}(x)$.

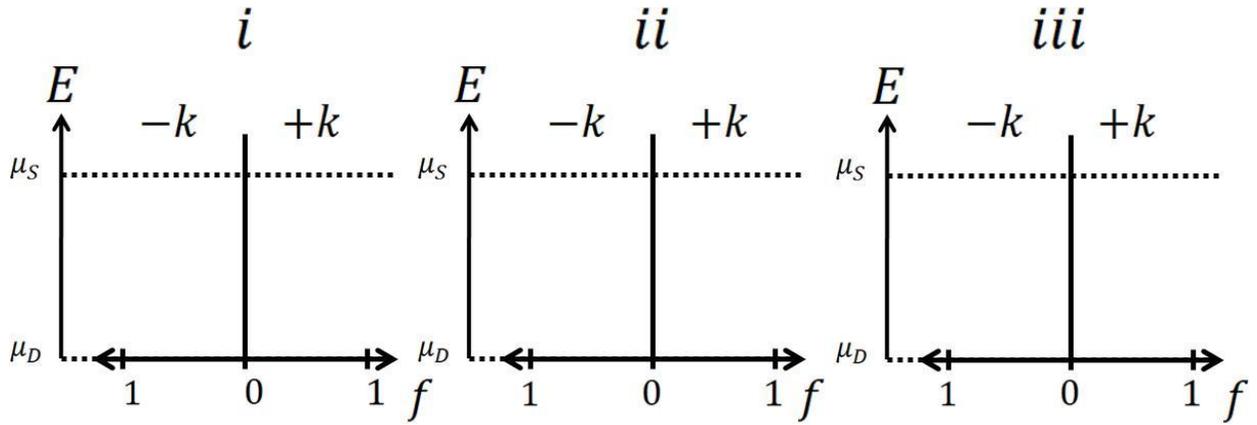
Question 4 This problem refers to the ballistic 1-D wire below. The X's in the wire are representative of elastic scattering sites, each with transmission, T . Assume $E_C < \mu_S, \mu_D$ where



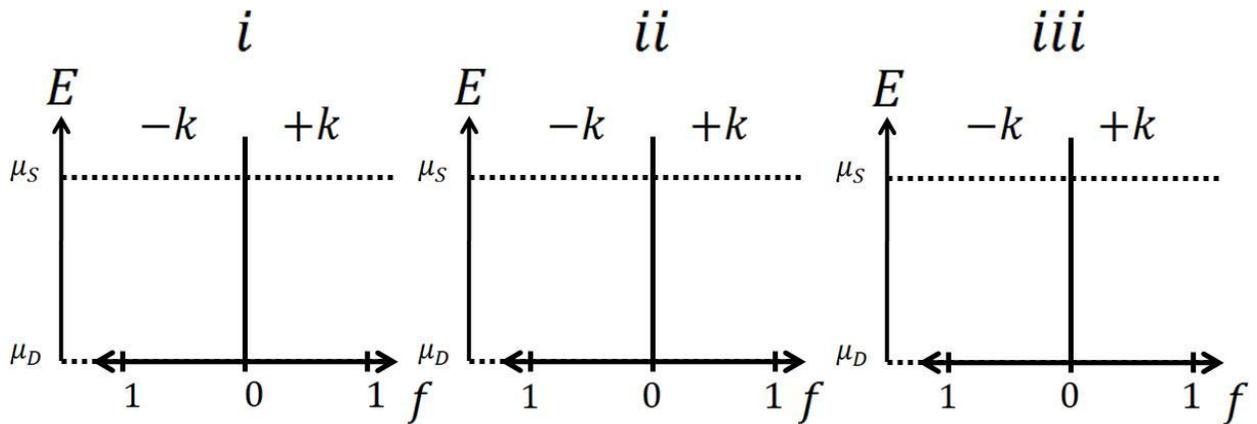
a) $T = 1.0$, plot the filling function at positions (i), (ii), and (iii) along the z-axis.



b) $T = 0.5$, plot the filling function at positions (i), (ii), and (iii) along the z-axis.

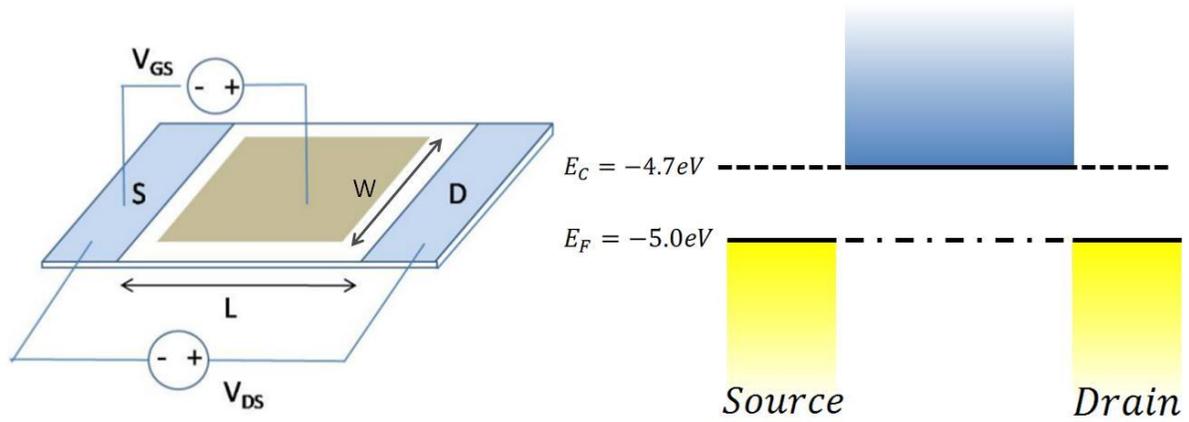


c) Consider a very large number of scattering sites along the wire. Plot the filling function at the source (i), at the midpoint of the wire (ii), and at the drain (iii).



Question 5 This problem refers to the 2-d quantum well FET. Assume the following:

$$T = 0\text{K}, L = 40\text{nm}, W = 120\text{nm}, C_G = 0.1\text{fF}, C_S = C_D = 0$$



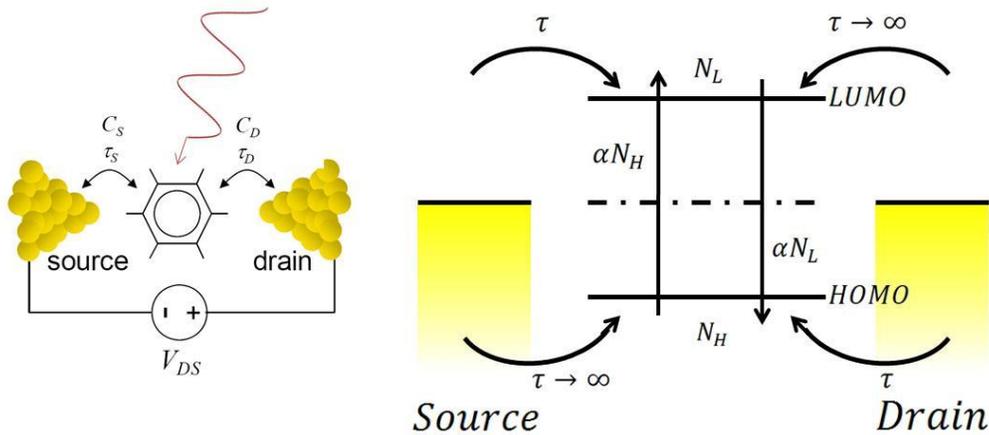
a) Compare the operation of the 2-D well in the ballistic and semi-classical regimes.

Assume $C_Q \rightarrow \infty \gg C_{ES}$ in both regimes. Take $\mu = 300 \frac{\text{cm}^2}{\text{V}\cdot\text{s}}$ in the semi-classical regime. Plot I_{DS} vs. V_{DS} for $V_{GS} = 0.5\text{V}$ and $V_{DS} = 0$ to 0.5V .

b) Explain the difference in the IV curves. Is there a problem with the theory? If so, what?

Question 6 (6.719 only) The following problem considers a 2-terminal conductor under illumination. The light produces an electron transfer rate of αN_H from the HOMO to the LUMO. The light also causes an electron transfer rate of αN_L from the LUMO to the HOMO, where α is proportional to the intensity of the illumination, and the electron populations in the LUMO and HOMO are N_L and N_H , respectively.

Assume $C_S = C_D$, that the LUMO and HOMO are delta functions, and $T = 300\text{K}$. Also, assume that under equilibrium in the dark, $E_F = \frac{E_L - E_H}{2} + E_H$.



Next, imagine that the contacts are engineered to have the following characteristics:

$$\text{Transfer rate between Drain and HOMO} = \frac{1}{\tau}$$

$$\text{Transfer rate between Drain and LUMO} = 0$$

$$\text{Transfer rate between Source and HOMO} = 0$$

$$\text{Transfer rate between Source and LUMO} = \frac{1}{\tau}$$

a) Determine the short circuit current for this system. (*i.e.* let $V_{DS} = 0$, what is the current that flows through the external short circuit?)

b) Determine the open circuit voltage for this system. (*i.e.* Disconnect the voltage source, what is the voltage that appears across the terminals of the molecule?)

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