ECE 4070/MSE 5470: Physics of Semiconductor and Nanostructures

Spring 2015

Homework 7   **Due on April 20, 2015 at 5:00 PM**

Suggested Readings:
a) Lecture notes

Problem 7.1 (The deep-acceptor problem and the 2014 Physics Nobel Prize)

Magnesium is a relatively "deep acceptor" in the wide bandgap semiconductor GaN. The acceptor ionization energy is $E_A \sim 160$meV. Consider a GaN sample (E_g=3.4 eV, $m_c \sim 0.2 m_0$, $m_v \sim 1.4 m_0$) doped with $N_A = 10^{18}$/cm^3 of Magnesium atoms. In the process of doping this sample with Magnesium, unintentional donors of density $N_D = 10^{14}$/cm^3 (E_D=10meV) also incorporate into the semiconductor.

a) Find the Fermi level E_f in the semiconductor at T=300K.

b) For T=300K, Plot n, p, N_A^-, N_D^+, $n+ N_A^-$, and $p+N_D^+$ as a function of the Fermi level E_F. Remember the Fermi level can be within the gap or in the conduction or valence bands. Therefore choose values of E_F from below E_V to above E_C. Indicate in the plot where the real Fermi level at 300K is. Explain.

c) Indicate the donor and acceptor ionization energies in your figure.

d) What are the densities and types of mobile carriers in the sample at 300K? Is the sample n- or p-type?

e) Do an online research of the connection between the p-type doping problem of wide-bandgap semiconductors and the 2014 Physics Nobel prize award.

Problem 7.2 (Time-dependent Effective Mass Equation)

Sometimes, for example when the external potential is time-dependent, time-dependent solutions are sought. Suppose the external potential is time-dependent and is $U(\vec{r}, t)$. We want to solve the time-dependent Schrodinger equation,

$$\left[\hat{H} + U(\vec{r}, t)\right]\psi(\vec{r}, t) = i\hbar \frac{\partial \psi(\vec{r}, t)}{\partial t}$$

Suppose we assume a solution for electron state near wavevector $\vec{k}_o$ based on a time-dependent envelope function,

$$\psi(\vec{r}, t) = \phi(\vec{r}, t)\psi_{n, \vec{k}_o}(\vec{r})$$

The underlying assumption for the above form of the solution is that the applied potential is slowly varying both in space and time so that the electron does not transition to another band. Then, following exactly the same steps as in the lecture notes, the envelope function can be shown to satisfy the time-dependent effective mass equation,

$$\left[E_n\left(\vec{k}_o - i\nabla\right) + U(\vec{r}, t)\right]\phi(\vec{r}, t) = i\hbar \frac{\partial \phi(\vec{r}, t)}{\partial t}$$

a) Consider the case when a uniform DC electric field is applied so that,

$$U(\vec{r}) = e\,\vec{E}.\,\vec{r}$$

Although the potential is time-independent we seek a time-dependent solution by solving the time-dependent effective mass equation. Find $\phi(\vec{r}, t)$ that satisfies,

$$\left[E_n\left(\vec{k}_o - i\vec{\nabla}\right) + e\vec{E} \cdot \vec{r} \right] \phi(\vec{r}, t) = i\hbar \frac{\partial \phi(\vec{r}, t)}{\partial t}$$

subject to the initial condition,

$$\psi(\vec{r}, t = 0) = \psi_{n, \vec{k}_o}(\vec{r}) \qquad \text{or} \qquad \phi(\vec{r}, t = 0) = 1$$

And show that your solution indeed satisfies the time-dependent effective mass equation.
Hint: look back at your earlier handout on electron dynamics in an applied uniform DC electric field.

b) The time-dependent solution found in part (a) has a time-dependent energy $E(t)$. What is it?

Problem 7.3 (Probability currents for the Effective Mass equation)

Consider a material with the conduction band dispersion given by,

$$E_c(\vec{k}) = E_c + \frac{\hbar^2 (k_x - k_{ox})^2}{2m_x} + \frac{\hbar^2 (k_y - k_{oy})^2}{2m_y} + \frac{\hbar^2 (k_z - k_{oz})^2}{2m_z}$$

a) Show that the plane wave envelope function,

$$\phi(\vec{r}) = e^{i\left(q_x x + q_y y + q_z z\right)} \qquad\qquad \psi(\vec{r}) = \phi(\vec{r}) \psi_{c, \vec{k}_o}(\vec{r})$$

is a solution of the effective mass equation with $U(\vec{r}) = 0$,

$$\left[\hat{E}_c\left(\vec{k}_o - i\vec{\nabla}\right) + U(\vec{r}) \right] \phi(\vec{r}) = E \, \phi(\vec{r})$$

b) Show that with $U(\vec{r}) = 0$, the complete solution $\psi(\vec{r})$ is a Bloch function (i.e. satisfies the Bloch's theorem) and has a crystal momentum equal to $\vec{k} = \vec{q} + \vec{k}_o$. Note that in the absence of any external potential the solution must necessarily satisfy Bloch's theorem and must be a Bloch state.

c) Find the probability current vector associated with the plane wave envelope function of part (a). Note that the probability current is given by a vector with x,y, and z components.

Problem 7.4 (A Quantum Well in a Semiconductor Heterostructure)

Consider a 80 Angstroms thick quantum well (i.e. $L = 80A$), as shown below. Suppose that $\Delta E_c = 150 \text{ meV}$. The conduction band dispersion relations are as follows:

Well: $E_{c1}(\vec{k}) = E_{c1} + \frac{\hbar^2 k_x^2}{2m_{x1}} + \frac{\hbar^2 k_y^2}{2m_y} + \frac{\hbar^2 k_z^2}{2m_z}$

Barrier: $E_{c2}(\vec{k}) = E_{c2} + \frac{\hbar^2 k_x^2}{2m_{x2}} + \frac{\hbar^2 k_y^2}{2m_y} + \frac{\hbar^2 k_z^2}{2m_z}$
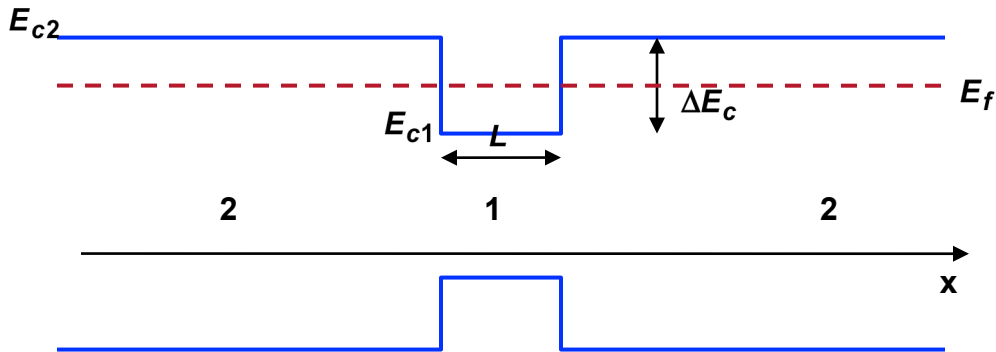
where:

$m_z = 0.10\, m_o$

$m_y = 0.045\, m_o$

$m_{x1} = 0.067\, m_o$

$m_{x2} = 0.20\, m_o$

a) How many conduction band bounds states are there in the quantum well? Analysis done in the lecture notes will not apply directly since the masses in the x-direction are different in the well and barrier materials.

b) Find the quantized energies relative to the conduction band edge E_{c1} of all the bound states in meV units? You will have to numerically or graphically solve this part.
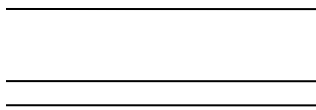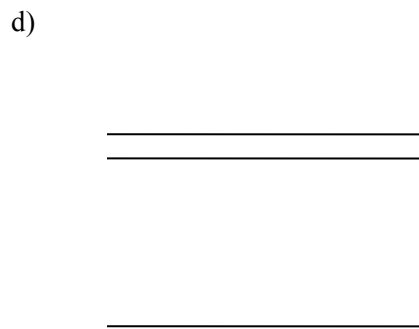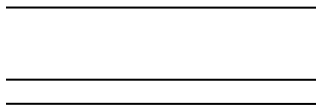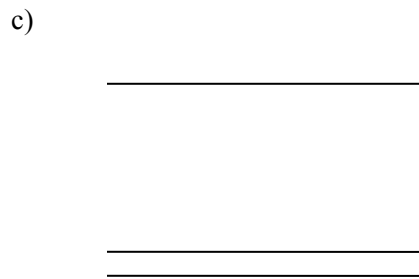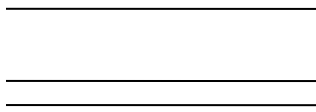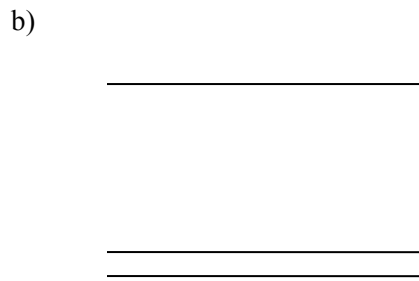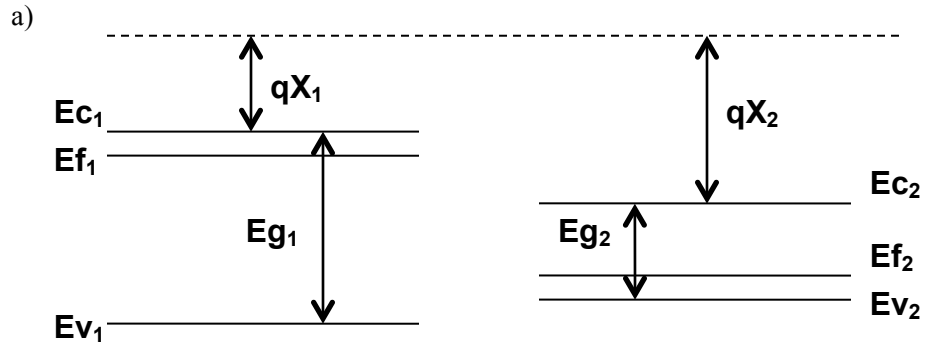
c) Suppose the position of the Fermi level E_f is known. Using your results from parts (a) and (b), write an expression that relates the total electron density n (units: #/m²) in the quantum well to the Fermi level. There should be no unevaluated integrals in your answer. **Hint:** The following integral might prove helpful:

$$\int_{E_a}^{\infty} dE \; \frac{1}{1+e^{(E-E_f)/KT}} = KT \log\left[1 + e^{(E_f - E_a)/KT}\right]$$
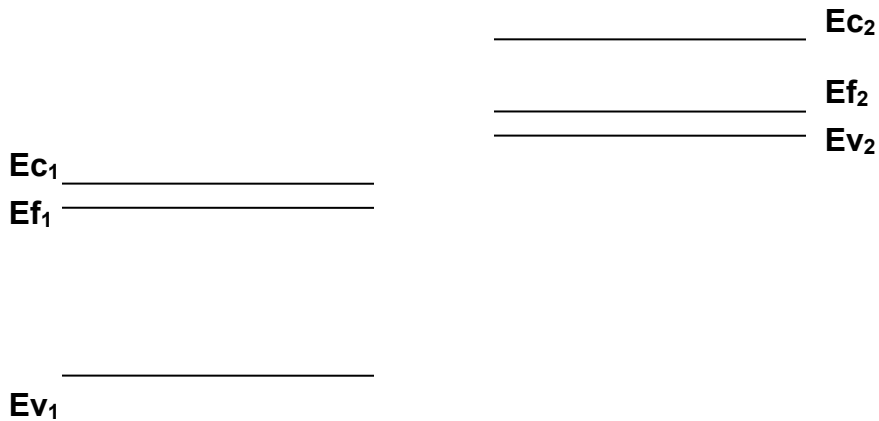
d) Suppose somebody tells you that the total electron density in the quantum well is 10^{16} 1/m². Find the position of the Fermi level with respect to the conduction band edge (i.e. find $E_f - E_{c1}$) in meV units. Assume room temperature. You might have to solve this part numerically.

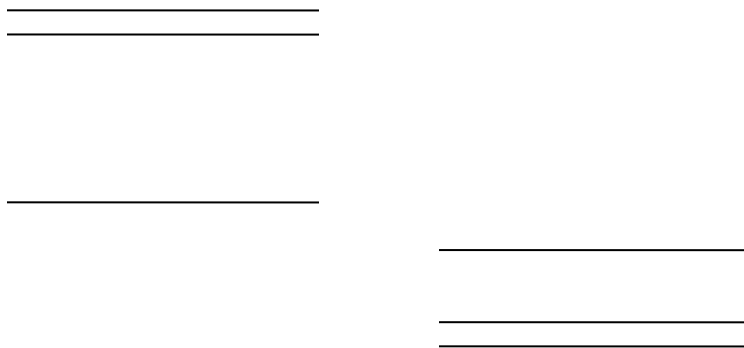## Problem 7.5 (Equilibrium in Semiconductor Heterojunctions with various band offsets)

In each of the parts given below band diagrams of two different semiconductors are drawn (one on the left side and the other on the right side). In each case you are supposed to **sketch** the **equilibrium** band diagram when a heterojunction is formed between the two semiconductors. In each case indicate the **depletion** and/or **accumulation** and/or **inversion** regions that may exist in equilibrium on either side of the heterointerface. For your convenience, I have already taken the liberty of aligning the band diagrams such that the alignment shown corresponds to the electron affinity rule (as shown explicitly in part (a)). All the labels are also shown in more detail in part (a), and which you can use for the other parts as well.

3

a)

Ec₁
Ef₁

qX_1

Eg_1

Ev₁

qX_2

Eg_2

Ec₂
Ef₂
Ev₂

b)

c)

d)

4

e)

E_{c2}

E_{f2}

E_{v2}

E_{c1}

E_{f1}

E_{v1}

f)

Problem 7.6 (Bloch transport and Bloch Oscillations)

The bandstructure of a fictitious 2D crystal with a square lattice (of lattice constant a is given by

$$E(k_x,k_x) = -E_0[\cos(k_x a) + \cos(k_y a)]$$

a) Make a semi-quantitative plot of the constant energy contours in the 1st BZ, and highlight the energies $E = 0, \pm E_0$.

b) Make a semi-quantitative plot of the effective mass in the (1,0) or k_x-direction, and in the (2,1) directions of the 1st BZ.

c) An 'electron' is initially 'located' at the Γ point $\mathbf{k} = (k_x, k_y) = (0,0)$ in k-space, and $\mathbf{r} = (x,y) = (0,0)$ in real space. Argue why this state cannot be an electron in an energy eigenstate of the 2D crystal, but a wave-packet. At $t = 0$, a force $\mathbf{F} = (F_x, F_y)$ from an electric field is turned on. The force points in an oblique direction such that $F_x = 2F_y$. Show the $\mathbf{k}$-space trajectory of the electron through the 1st BZ, including Umklapp processes, for the time interval $0 \le t \le 4T$, where $T = \pi\hbar / aF_x$.

d) Calculate and plot the x- and y-components of the velocity and position of the electron, all as functions of time for $0 \le t \le 4T$.

e) Make a graph of the trajectory of the electron in the real (x,y) space. Explain the phenomena.

f) We discussed in class that electrons in typical semiconductors do not exhibit Bloch oscillations because the BZ edge is too far in k-space; electrons scatter before they make it to the BZ edge. Can you suggest a way around this problem?