Solid State Devices I - Purdue ECE-606

Homework No. 2

Student name: _____

Student ID: _____

I solved the homework assignment myself without copying a solution from someone else or from the web. Student Initials here: _____

Introduction

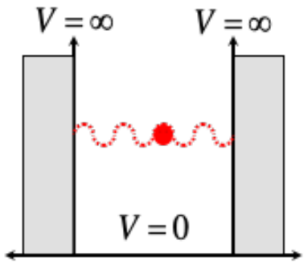
The project you will be working on in a couple weeks is about quantum dot optical transitions. This problem set serves as an introduction to the fundamental principles of optical transitions in quantum systems. The one-dimensional infinite potential well in problem 1 is a simplified model of a quantum dot, and it demonstrates two key principles of optical transitions:

1. **Energy Conservation**: Photon absorption or emission can only occur if the photon's energy, $h\nu$, is equal to the energy difference between the initial and final states of the electron, i.e., $\Delta E = |E_f - E_i|$.
2. **Selection Rules**: In this exercise you will calculate the "strength" of transitions induced by light. You will find that some values are finite, and others are zero. These are related to allowed and forbidden (verboten) transitions.

By working through this problem, you will be able to perform "back-of-the-envelope" calculations for light-matter interaction at the quantum level, which comes in handy for project 1.

Problem 1: Optical Matrix Elements in a 1D Infinite Square Well (20 points total)

Consider a particle of mass m^* confined within a one-dimensional infinite square well of length L, centered at the origin (from $x = -L/2$ to $x = L/2$).



The energy eigenvalues and corresponding wavefunctions for this system are given by:

$$E_n = \frac{\pi^2 \hbar^2}{2m^*} \frac{(n+1)^2}{L^2}$$

and

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{(n+1)\pi(x + L/2)}{L}\right)$$

These expressions use the convention where the ground state is indexed as $n = 0$.

We are interested in optical transitions induced by an electric field oscillating in the x-direction. If the optical wavelength (green light for example is 514nm) is much larger than the length of electronic wavefunction and charge distribution (~ 5-10nm), then the strength of these transitions can be very well described by the so-called **dipole approximation**.

$$\mu_{i \to f} = A \int_{-L/2}^{L/2} \psi_i(x) \cdot x \cdot \psi_f^*(x) dx$$

Here, $\mu_{i \to f}$ is the optical matrix element, i and f represent the initial and final states, respectively, and "*" indicates the complex conjugate in the case of complex wavefunctions.

a. Derive a general analytical expression for the optical matrix element, $\mu_{i \to f}$, for any initial state i and final state f. Leave the constants A and L in the analytical expression. (8 Points)
b. Sketch the wavefunctions $\psi_i(x)$ and $\psi_f(x)$ along with the integrand of the matrix element, $\psi_i(x) x \psi_f(x)$, for the following transitions:
   - $i = 0 \rightarrow f = 1$
   - $i = 0 \rightarrow f = 2$

Analyze the symmetry of each component (initial state, final state, and the product) using the terms "even function" and "odd function". Based on the symmetry of the integrand, explain the expected value of the integral for each case and thus comment on whether the optical transition is allowed or forbidden. (10 Points)

c. From the analytical expression in (a) and examples in (b), a certain set of transitions take on a very specific value. Such condition is historically referred to as "verboten." Create a matrix showing the optical transitions from initial states (rows) to final states (columns) from $n = 0$ to $n = 7$. Indicate which transitions are allowed and which are forbidden, and identify a general selection rule for optical transitions in this system. (2 Points)

I \ F	0	1	2	3	4	5	6	7
0								
1								
2								
3								
4								
5								
6								
7								

Problem 2. (28 points total)

This problem extends the concepts of a one-dimensional quantum well to a more complex, **three-dimensional (3D) system**. You will analyze the optical transitions of a particle confined within a 3D rectangular box. The particle's quantum state is now described by three quantum numbers, (n_x,n_y,n_z). Consequently, the optical transitions are governed by a vector of matrix elements, $\vec{\mu}_{i,f}$, with components for each spatial direction: μ_x, μ_y, and μ_z.

The wavefunction for a particle in this 3D box is given by:

$$\psi_{n_x,n_y,n_z}(x,y,z) = \sqrt{\frac{8}{L_x L_y L_z}} \sin\left(\frac{\pi}{L_x}(n_x+1)\left(x+\frac{L_x}{2}\right)\right) \sin\left(\frac{\pi}{L_y}(n_y+1)\left(y+\frac{L_y}{2}\right)\right) \sin\left(\frac{\pi}{L_z}(n_z+1)\left(z+\frac{L_z}{2}\right)\right)$$

where the confinement ranges are:

$$-\frac{L_x}{2} \le x \le \frac{L_x}{2}, \quad -\frac{L_y}{2} \le y \le \frac{L_y}{2}, \quad -\frac{L_z}{2} \le z \le \frac{L_z}{2}$$

The initial and final states are defined by their quantum number vectors:

$$\vec{\imath} = \{i_x, i_y, i_z\} \quad \text{and} \quad \vec{f} = \{f_x, f_y, f_z\}$$

The optical matrix element for the x-polarization is:

$$\mu_{x,i,f} = A \int_{-L_x/2}^{L_x/2} \int_{-L_y/2}^{L_y/2} \int_{-L_z/2}^{L_z/2} \psi_{i_x,i_y,i_z}(x,y,z) \cdot x \cdot \psi^*_{f_x,f_y,f_z}(x,y,z)\, dx\, dy\, dz$$

The components $\mu_{y,i,f}$ and $\mu_{z,i,f}$ are analogous.

The norm of $\mu_{i,\vec{f}}$ is

$$\left|\mu_{i,\vec{f}}\right| = \sqrt{\mu^2_{x,i,\vec{f}} + \mu^2_{y,i,\vec{f}} + \mu^2_{z,i,\vec{f}}}$$

a. Derive a general analytical expression for each of the optical matrix elements, μ_x, μ_y, and μ_z, for an arbitrary initial state i and final state f. Utilize the principle of separation of variables and your results from Problem 1 to solve the integrals. Leave the constants A and L in the analytical expression (8 points)
b. Calculate a general expression for the transition energy, $\Delta E_{f\to i} = E_f - E_i$. Normalize your expression by the energy scale $E_{norm} = \frac{\pi^2\hbar^2}{2m^* L^2}$. (2 points)
c. Consider a specific system with parameters: m^*=0.04 (in units of electron mass) and L=3 nm. Assume L_x=4L, L_y=6L, and L_z=2L. Calculate all possible transitions from the three lowest energy states—the ground state (0,0,0) and the first two excited states (1,0,0) and (0,1,0)—to all possible final states with quantum numbers {nx} ∈ {0,1,2,3,4,5,6,7,8,9}, {ny} ∈ {0,1,2,3,4,5,6,7,8,9}, and {nz} ∈ {0,1,2,3}.

Use Excel or the programming language of your choice, for each of the 1200 transitions:

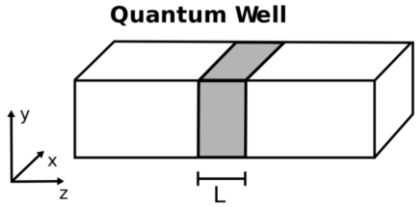
1. Explicitly compute the transition energy $\Delta E_{i \to f}$ in electron-volts (eV).
2. Explicitly compute the individual optical matrix elements, μ_x, μ_y, and μ_z.

Lastly, identify and list the number of allowed transitions (those where $\left|\mu_{i \to f}\right| \neq 0$) that fall within the energy range of 0 to 1 eV. (15 points)

d. The prior calculations indicate that only few optical matrix elements are non-zero. Speculate what realistic conditions might change that and "turn-on" more optical transitions to have a finite optical matrix element. (3 points)

Problem 3. (7 points total)

This problem expands on the concepts of optical transitions to a different confinement geometry: a **Quantum Well** (https://en.wikipedia.org/wiki/Quantum_well).



Unlike a quantum dot which confines a particle in all three dimensions, a quantum well confines a particle in only one dimension (here, $-\frac{L}{2} \leq z \leq \frac{L}{2}$), while allowing it to move freely in the other two (the x-y plane). This leads to a new set of wavefunctions and matrix elements.

The model assumes an infinitely large plane in the x and y directions, with a finite thickness L in the z-direction. This results in a discrete quantum number in the z-direction and continuous quantum numbers in the x and y directions.

$$\vec{\imath} = \{k_{xi}, k_{yi}, i_z\},\ \vec{f} = \{k_{xf}, k_{yf}, f_z\}$$

The initial and final wavefunctions for a particle in this system are given by:

$$\psi_{i_z,k_{xi},k_{yi}}(x,y,z) = \sqrt{\frac{2}{L_x L_y L}} \exp(-jk_{xi}x) \exp(-jk_{yi}y) \sin\left(\frac{(i_z+1)\pi\left(z+\frac{L}{2}\right)}{L}\right)$$

$$\psi_{f_z,k_{xf},k_{yf}}(x,y,z) = \sqrt{\frac{2}{L_x L_y L}} \exp(-jk_{xf}x) \exp(-jk_{yf}y) \sin\left(\frac{(f_z+1)\pi\left(z+\frac{L}{2}\right)}{L}\right)$$

where $j = \sqrt{-1}$.

The corresponding energy is:

$$E_{n,k_x,k_y} = \frac{\hbar^2}{2m^*}\left(k_x^2 + k_y^2 + \frac{\pi^2(n+1)^2}{L^2}\right)$$

The optical matrix element for the x-polarization is:

$$\mu_{x,i,\vec{f}} = A \int_{-L_x/2}^{L_x/2} \int_{-L_y/2}^{L_y/2} \int_{-L/2}^{L/2} dx\ dy\ dz\ \psi_{i_z,k_{xi},k_{yi}}(x,y,z) \cdot x \cdot \psi^*_{f_z,k_{xf},k_{yf}}(x,y,z)$$

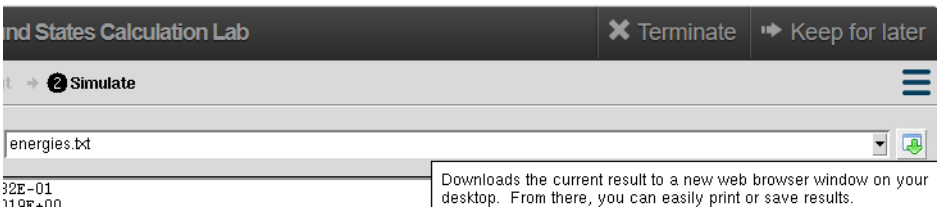
In this simplified problem, assume that the initial and final in-plane momentum quantum numbers are the same, i.e., $k_{xf} = k_{xi}$ and $k_{yf} = k_{yi}$. This corresponds to the physical condition that photons do not transfer significant momentum.

a. Calculate the optical matrix elements in the X, Y, and Z directions, leveraging the given wavefunctions and the simplification for the momentum quantum numbers. Leave the constant A in the analytical expression (5 points)
b. Based on your calculations and understanding of optical transitions, hypothesize on the consequences of optical absorption/emission in Quantum Wells versus Quantum dots. Consider the geometry and the nature of the wavefunctions in each case. (2 points)

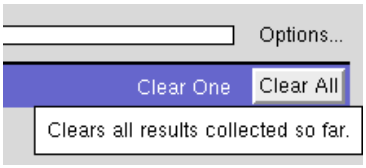
Problem 4 (25 points total)

Use the "Bound States Calculation Lab" on nanoHUB (https://nanohub.org/resources/4875), Jupyter (https://nanohub.org/resources/jupyter), Matlab (there is a Matlab module in Jupyter), or alike, as well as analytical methods to solve this homework problem.

a. Write down the analytical expressions for the eigenvalues and wavefunctions of an electron in a one-dimensional infinite square well. Then, using these expressions, calculate the first 10 eigenvalues for an electron with an effective mass of 0.067 inside a 10 nm wide infinite square well. (2 points)
b. Using the Bound States Lab, calculate the eigenvalues and wavefunctions for an electron with an effective mass of 0.067 in a square well of 10 nm width and a 0.4 eV barrier height. From the simulation results: (2 points)
   - Determine the number of wavefunctions confined within the well and list the discrete energies of these states. (you can download the energies by clicking on the green download button on the top right of the app window)

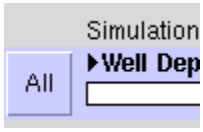


   - Export the magnitude squared of the eigenstates as a function of distance. You will need to use the first and second column of the output "magsqrd_wavefunction_vs_distance.txt" for the later exercises.
c. Repeat the numerical calculation from (b) for five additional barrier heights: 0.1 eV, 0.2 eV, 0.8 V, 1.6 eV, and 3.2 eV. Analyze the energies and the wavefunctions: (8 points)
   - Plot the ground state energies as a function of the total barrier height (the barrier height on the x axis and the energy on the y axis). Add to the plot the value of the analytical result obtained in (a) as a horizontal line. Interpret the trend observed in the plot.
   - Re-plot the results on a semi-log scale (set the barrier height to log scale). Can you clarify the trend you described before?
   - Integrate the 6 ground state wavefunctions from the exported data (use Jupyter, Matlab, Octave, or alike).
   - Validate that the wavefunctions are normalized to 1.0. If not, correct your code.
   - Compute the wavefunction portions that are within the potential barrier, and create two "wavefunction percentages vs barrier height" charts (on linear and semi-log scale). How do the results relate to the analytical expression?
d. Clear all previous results with the "Clear All" button and generate new simulations. Simulate the following potential wells: (5 points)



- Square Well: mass 0.067, width 10 nm, barrier height 2 eV
- Parabolic Well: Oscillator Energy 0.2 eV
- Triangular Well: Electric Field 5e7 V/m
- V-Shaped Well: Electric Field 1e8 V/m

- For each potential well calculation, export the images of "Potential vs. Distance" and the text results of "energies.txt", into your solution.
- Click the "All" button in the "Potential vs. Distance" output. Export the image of this combined plot. Compare the results



- Clear the Square Well and Parabolic Well results by clicking "Clear One." Export a new plot showing only the Triangular and V-Shaped Well results as an image and comment on the results.

e. Using results from (d), calculate the first 5 energy gaps between the eigen energies for the four different potential wells. (8 points)

$$\Delta_1 = E_2 - E_1$$
$$\Delta_2 = E_3 - E_2$$
$$\ldots\ldots$$
$$\Delta_5 = E_6 - E_5$$

Compare the energy gaps using line plot and comment and interpret the results.