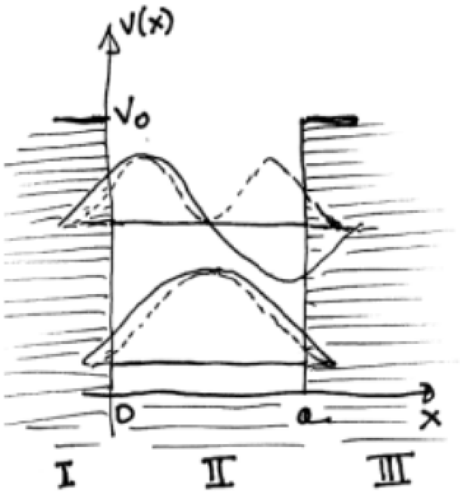
Option I:

Semiconductor's Quantum Well



3rd Year of the Degree in Physics

Electronic Physics

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May 10^{th} 2025

Contents

Figures Index

1 Introduction

This project aimed to simulate the quantum energy levels of an electron confined within a semiconductor quantum well using Python. The results obtained are presented below, together with direct answers to the questions posed in the class assignment.

2 Results

These are the results of calculating the energy spectrum of a semiconductor with a width of $a = 3\text{Å}$ and a potential height of $V_o = 3\text{eV}$. First, we will show the plot of the energy spectrum and describe the calculation process in general terms. The full code will be provided in the assignment so that it can be reviewed in more detail.

2.1 Plot of the energy spectrum of the potential and calculation of the first two allowed energy levels

In order to obtain the first allowed energy levels, we used the Newton-Raphson method to find the values of z satisfying the following equations.

For the odd functions:

$$z \tan z + \sqrt{\left(\frac{z_o}{z}\right)^2 - 1} = 0$$

For the even functions:

$$z \cot z + \sqrt{\left(\frac{z_o}{z}\right)^2 - 1} = 0$$

Once the roots satisfying the equations are found, the corresponding energy levels can be calculated using the following expression:

$$E = \frac{\hbar^2 \chi^2}{2 m_{\text{eff}} a^2}$$

where χ are the roots, and m_{eff} is the effective mass of the electron, which we adjust to simulate the behavior of the electron inside the semiconductor. Using this formula, we obtain the following energy levels:

$$E_1 = \frac{\hbar^2 \chi_1^2}{2 m_{\text{eff}} a^2} = 5.380 \times 10^{-80}\ \text{J}$$

$$E_2 = \frac{\hbar^2 \chi_2^2}{2 m_{\text{eff}} a^2} = 1.109 \times 10^{-79}\ \text{J}$$

Finally, the plot of the energy levels is the following.

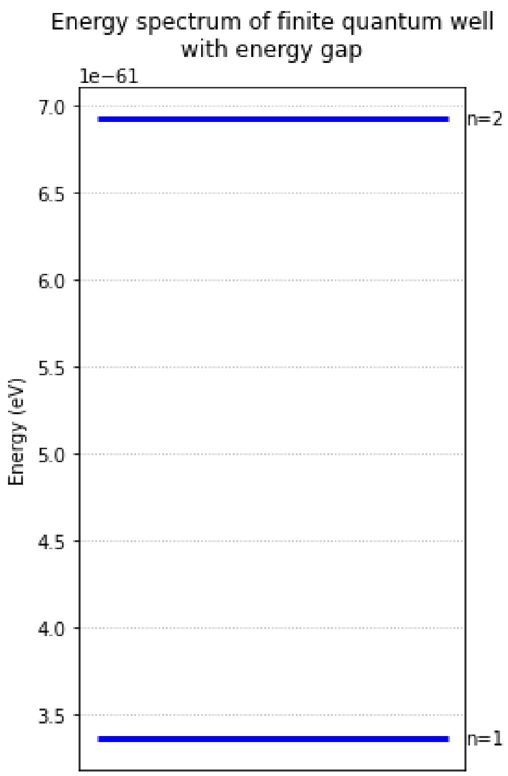

Figure 1: Energy bands plot

2.2 Find the correct effective mass

In order to obtain the previous results, we had to adjust the effective mass so as to obtain the correct energy levels. The effective mass is the variation of the mass of the electron due to its interaction with the semiconductor lattice. It can be calculated with this expression:

$$m_{eff} = xm_e$$

Where m_e is the mass of the electron and x is the parameter to adjust. Because this is a simulated case and not a real experiment, it must be adjusted manually. We have found that the energy levels showed before are obtained with $x = 0.8$ giving an effective mass of, $m_{eff} = 7.28719 \times 10^{-31} kg$.

2.3 Relationship between energy levels and the depth of the potential well.

When the electron's energy is below the potential of the well, its wave function becomes an exponential decay. This is why the electron cannot escape the well: the probability of finding the electron outside the well decreases so rapidly with distance. The greater the potential, (1) the more energy levels experience this phenomenon, (2) the faster this probability decays, and consequently, (3) the less likely quantum tunneling becomes.