Computational Lab 2: Quantum wells

In this computational assignment, you will be provided with pre-written Matlab codes for an iterative solver which couples the Poisson and Schrodinger equations to examine quantum wells which have been formed using heterojunctions.

The Matlab code files required for this assignment are available in the "Computational Lab Assignment 2" folder on the PHY4MES Moodle site.

In this lab assignment, you will use Matlab to add to/edit the provided scripts. For those who are unfamiliar with Matlab and/or in need of a refresher, it is recommended that you complete the Matlab tutorial made available on Moodle before attempting this assignment. You may find that to complete this assignment you will need to consult the help documentation in Matlab or available online from http://au.mathworks.com/help/matlab/

You are expected to submit an electronic copy of the following on Moodle:

- ❑ A .m file containing your code for calculating and plotting the energy levels of an infinite potential quantum well as a function of quantum number, as well as a file (.doc/.docx/.pdf) containing your graph and answer to the question (Section 2, Part A)
- ❑ A file (.doc/.docx/.pdf) containing your plots and discussion for the single quantum well (Section 2, Part B)
- ❑ A file (.doc/.docx/.pdf) containing your plots and discussion for the double quantum well (Section 2, Part C)
- ❑ A file (.doc/.docx/.pdf) containing your plots and discussion for the triple quantum well (Section 2, Part D)

You may combine all of your text documents into a single file; however, make sure you clearly indicate where each section starts and ends.

You must submit any and all .m files you produce for this assignment.

Be advised that your work may be analysed using Turnitin to check for plagiarism.

Summary

Quantum wells in semiconductor heterostructures are interesting and technologically useful structures, and one of the few ways in which truly quantum confined electrons can be realised. These quantum wells are typically produced either by physically restricting the dimensions of a semiconductor, as in the case of quantum dots, or by utilising the band offsets between various semiconductor materials and modulation doping, which results in the accumulation of electrons in an energetic minimum. This latter approach is widely used for AlGaAs/GaAs/AlGaAs quantum well structures, which can be routinely grown in controlled layers by using Molecular Beam Epitaxy. In this lab, you will experiment with layered quantum well structures by controlling both the thickness and the energy level structure of each layer.

This lab has several parts; all are based on similar codes and concepts.

In **part A**, you will write a script to perform a simple calculation based on a one-dimensional infinite potential well, and plot the results.

For **parts B, C and D**, you are provided with code which performs iterative calculations using the coupled Poisson-Schrodinger equations. This means that an initial guess of the quantum well potential is used to generate the quantum eigenstates, which are in turn occupied, after which the code recalculates the potential and repeats the process until the change in potential drops below a pre-set threshold. Solvers such as this are used widely in research programs which are aimed at developing semiconductor quantum structures. You will alter the provided code and plot the calculated quantities.

Here be the assignment

Part A

An electron confined in a one-dimensional infinite potential well of width *W* has energy eigenvalues

$$E_n = \frac{h^2 n^2}{8 m_e W^2}$$

1. Write a script which calculates the first ten energy levels (n from 1 to 10) of an electron confined to a quantum well. You should perform this calculation for a wells of width 3, 6, and 9 nm.
2. Plot the results of these calculations, overlaid on the same set of axes to enable direct comparison. Ensure that the *x* axis of your plot is *n* (the quantum number for the state), and that the *y* axis presents the energy eigenvalues in terms of electron volts.

How does changing the well width affect the electron energy eigenvalues?

You may find it useful to refer back to this graph during the other parts of this section.

Poisson-Schrodinger Solver

The scripts you will use for part B, C and D are all very similar in structure. You should read the following two pages carefully for important details on how to extract useful quantities from the calculations and how to usefully alter the scripts.

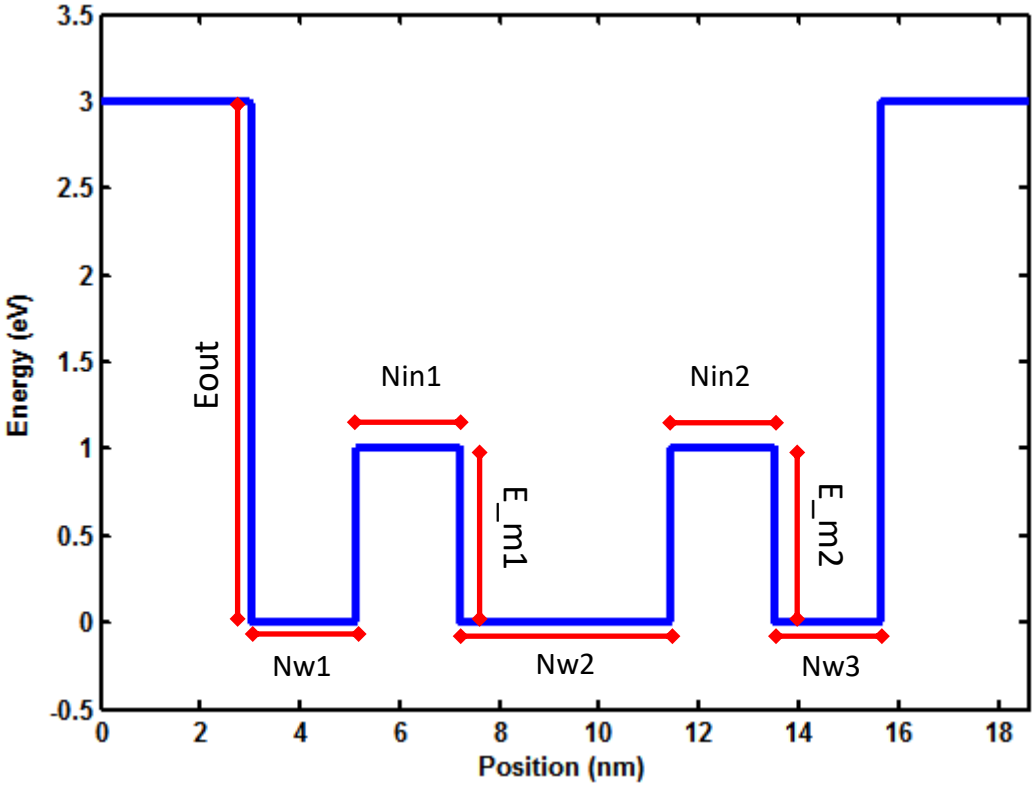
Warning: *These calculations may take some time. Matlab will display the calculated maximum difference between the potential matrices at each iteration, and the calculation will continue until this value reaches below the set tolerance (1e-6 by default). If you wish to abort a calculation, press CTRL+C.*

Inputs

The parameters which you should change to alter aspects of the calculation have been collected into a single area of the code, which begins at line 17 in the files QW_1.m, QW_2.m, and QW_3.m. Don't alter the names of these variables; they are called upon while the calculation is being performed. Changing the name of the variable will require you to rewrite large amounts of the code. Don't do this.

Variable	Units	Definition
a	m	Mesh point size
mu	eV	Fermi level, determined relative to the energy 0 of the bottom of the wells.
T	K	System temperature
Nout	None	Number of mesh points in the outer layer
Nin	None	Number of mesh points in the inner barrier layer (see below)
Nin1	None	Number of mesh points in the first (left) inner barrier layer (see below)
Nin2	None	Number of mesh points in the second (right) inner barrier layer (see below)
Nw1	None	Number of mesh points in the first quantum well (see below)
Nw2	None	Number of mesh points in the second quantum well (see below)
Nw3	None	Number of mesh points in the third quantum well (see below)
E_m	eV	Energy height of the internal barrier layer
E_m1	eV	Energy height of the first (left) internal barrier layer (see below)
E_m2	eV	Energy height of the second (right) internal barrier layer (see below)
E_out	eV	Energy height of the outer barrier

Below is a schematic diagram of the three-quantum-well structure, with each of the relevant parameters marked out. A diagram such as this can be produced by plotting `Ec` as a function of `XX` when you perform your calculation



The system is divided up into discrete mesh points, and equations (Poisson, Schrodinger) are solved at each point. The size of each object (barrier, well) is defined by the number of mesh points, multiplied by a scaling factor which converts the number of points to a physical length (X=Nw1*a).

Increasing the size of objects can therefore be accomplished either by changing the mesh point size, reducing the physical resolution but maintaining the time taken to perform the calculation, or

by increasing the number of mesh points assigned to a particular feature.

The second approach will maintain a constant physical resolution but may cause your calculation to take longer. Increase the number of mesh points rather than changing the mesh point size when you need to alter feature sizes.

We recommend:

- An outer barrier height (E_out) of 4 eV for all calculations, unless directed to change the outer barrier height
- A Fermi level position (mu) of 1 eV is recommended for default calculations
- Your individual well widths should stay in the range of 2nm to 20 nm, as should your barrier thicknesses.

Equations

There are no inputs you need to calculate for this code. You will need to code some calculations in order to retrieve important observable quantities. The following calculations are written as you would input the commands into Matlab, with 'x' used in place of numbers for the general case.

In general, you can replace the variable to the left of the equals sign with any other variable name you wish provided you are consistent. The following strings do not represent the only way of calculating/isolating each quantity, and you should feel free to use another method.

Wave Functions

The wavefunctions generated by this calculation are stored in the matrix P. Each column in the matrix is a separate wavefunction, with the wavefunction of the lowest energy state appearing in the first column. Therefore, the wavefunction (W in this case) of the x^{th} eigenstate can be accessed using the command:

```
W=P(:,x)
```

Probability density

Given that you can isolate the wavefunction of every system eigenstate, it is straightforward to generate the probability density for each eigenstate. The wavefunctions generated by this code are all real valued, so you simply need to square the wavefunction using element by element multiplication.

Energy Eigenvalues

The energy eigenvalues are stored in the output matrix D, which is a single column matrix. The lowest energy eigenstate of the system is the first element in the matrix. The x^{th} element of the matrix can be accessed using the command:

```
E=D(x)
```

Electron Density

The total electron density (nx_sum) in a particular eigenstate (x) can be calculated using the following combination of commands, replacing x with the number of the eigenstate of interest.

```
Occ_x=log(1+exp((mu-D(x))./kT))

Ed_x=P(:,x)*Occ_x*P(:,x)'
```

```
N_x=2*n0*Ed_x

nx_sum=1e-4*sum(sum(N_x.*[ones(Np,1)]))
```

This value (`Nx_sum`) is the number density of electrons, and not the charge density.

Potential

You can view the calculated potential by plotting `U1` as a function of `XX`.

Shape of quantum well

You can view the initial potential profile by plotting `Ec` as a function of `XX`. This, when added to U1, gives the final potential profile of the quantum well structure-essentially taking into account the distortion of the well structure due to the superimposed potential arising from the charge distribution in the well. This is calculated in the code as `U`.

You should check this shape after a calculation when you are answering questions; the induced potential will distort the dimensions of your quantum well.

Part B

In Part B you will be using the code QW_1.m, which simulates one finite potential quantum well.

Questions you should seek to address are:

- What effect, if any, does changing the energy barrier height (E_out) have on the electron energy eigenvalues and electron density of the eigenstates?
- What effect, if any, does changing the quantum well width (Nw) have on the electron energy eigenvalues and electron density of the eigenstates? Does the behaviour match what you see in the case of an infinite potential well?
- How does altering the system temperature change the number density of electrons in the occupied eigenstates? Is the observed behaviour what you expect?
- What effect, if any, does altering the Fermi level (mu) position have on the number density of electrons in the occupied eigenstates and the energy eigenvalues? Is the observed behaviour what you expect?
- What effect, if any, does changing the thickness of the barriers (Nout) while maintaining the same well size (Nw) have on the energy eigenvalues and electron density of the eigenstates?
- Is the probability density of the electrons confined purely to the quantum well, as it is in the case of an infinite potential well? Why/why not?

Part C

In Part C, you will be using the code QW_2.m, which simulates two coupled quantum wells separated by a barrier. You can independently set the width of each of the quantum wells and both the height and width of the middle barrier. This middle barrier does not have to be identical in height to the two outer barriers.

Begin by investigating the following:

- Does this calculation replicate the behaviour of the single quantum well solver (QM_1.m) when you set the width of the internal barrier (Nin) to 0?
- Setting the inner barrier to the same height as the outer barriers (ie E_m=E_out), the width of one well to 3nm and the other well to 5.1nm and the width of to 3nm (Nw1=100, Nw2=170 for default mesh point size), change the width of the inner barrier (Nin) for a few values between 2nm and 20 nm. If you plot the probability density for various eigenstates within each well as a function of position, you will note that the shape of the probability density may change with this change in inner width

due to an increase/decrease in the coupling between the wells. Noting which well the probability density is localised to will also let you to determine which well the wave function is an eigenstate for (if the coupling between wells is strong, the wave function may be an eigenstate of the whole system rather than just one/two wells). Does changing the barrier width have any effect on the energy eigenvalues and electron density?

- Setting the width of the inner barrier to 6nm and the width of each well to 3nm (Nw1=Nw2=100 for default mesh point size), investigate the effect of changing the height of the inner barrier (E_m). As with the previous exercise, changing the barrier height will modify the coupling between wells. Does changing the barrier height have any effect on the energy eigenvalues, electron probability distribution and electron density? Is there any difference if the Fermi level is set to above/below the inner barrier height?

Part D

Consider two quantum wells in GaAs/AlGaAs. Well A has a width L, and Well B has a width of 2L; the wells are separated by a large distance (the inner barrier) such that there is no significant coupling between the wells (ie the probability density from an eigenstate in one well does not significantly extend into the other well). It is possible to use infinite potential wells to investigate this situation and ignore the potential generated by the charge density in the well. However, the quantum wells in GaAs/AlGaAs heterostructures are typically quite shallow, and as we have seen the potential generated by a charge density in a quantum well can have a significant influence over the solutions.

From the electron affinity χ we can determine that these wells will have an initial depth of 0.33 eV. The .m file GaAs_solver.m is the same Poisson-Schrodinger solver code as QW_2.m, however it has the inner and outer barrier widths set to 0.33 eV, has a modified electron mass to represent the mass of electrons in GaAs, and has the relative permittivity set to 12.5, a compromise between the values for GaAs and AlGaAs to simplify the calculations. In this exercise, you will set up the same situation as the written assignment (widely separated quantum wells, well A with a width L, well B with width 2L, where L is between 2nm and 10 nm)

Use this solver and some quick calculations to investigate the following:

- Use the particle-in-a-box formula to determine L such that there are three quantum states with an energy less than 0.33 eV in well B. Use an electron mass of $0.067m_0$, appropriate for GaAs, for the calculation.
- Set the one well (A) in the code to the width you've calculated, the width of the other well (B) to double that value, and set the separation between the wells (the inner barrier width) to 10nm. Run the code. Are there three eigenstates within well B? Is there one eigenstate within well A? Is the probability density for each eigenstate with an energy less than 0.33 eV localised to one quantum well? Record the charge density for each eigenstate inside the wells.
- The previous calculation was performed with a chemical potential significantly higher than the well depth (1eV versus 0.33 eV). Taking the value of energy for the lowest eigenstate in well A from the previous calculation, set mu to three times that value (as in the written assignment) and run the code again. Compare the eigenvalues of the eigenstates within the well to those for the previous point. Compare the charge density for the eigenstates within the well to those for the previous point. Has there been a significant change? Increase the separation between the two wells
- Repeat for L even larger. What does this change about the number of states in each well and the charge density in those eigenstates? Briefly discuss how these observations might influence the choice of well width in GaAs/AlGaAs device architectures.