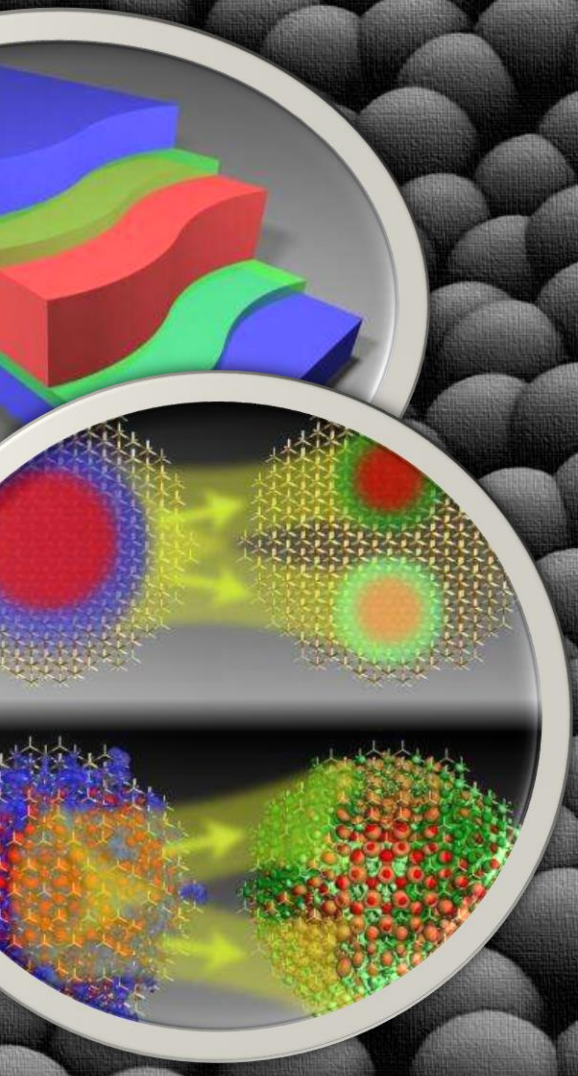
Computational Physics Lab (MP 408)

Project Report



Simulation of Quantum Well Structures

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Integrated M.Sc. Physics (IV) **Sem : 8th**

Subject : Experimental Techniques II

Computational Physics Lab

⋇ Mini Project ⋇

Simulation of Quantum Well Structures using Octave

By

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My Contribution to the Project

- In this project I have done the half of the coding part, that includes Animation of electron moving into the 3D quantum well of continuously decreasing length, the final designs and editing of the plots (The other half part of the coding that needed for these plots is done by my teammate Kavin Dave) so that user can understand the output more clearly.

- Further I have made the code such a way that if user don't have any input values and just want to see the results, user can use pre-defined values. And these pre-defined values (the values are collected by my team member Rahul Choudhury) are also user can see in the command window after run the code.

- In this final Report the flow chart you can see on the page no. 15 and the code on page no. 17 are edited by me.

- And finally, I have collected all the contributions (Quantum Confinement by Kavin Dave, Particle in box by Pujan Joshi, Applications by Zahabiyah Zaveri) from the teammates and merge them and create this final report.

Future Scopes of this Project

- I recently learn some more features of octave that includes the IO Dialog Boxes.
- In future to make it more user friendly I will replace all the IO operation that is currently working in command window with IO Dialog Boxes.

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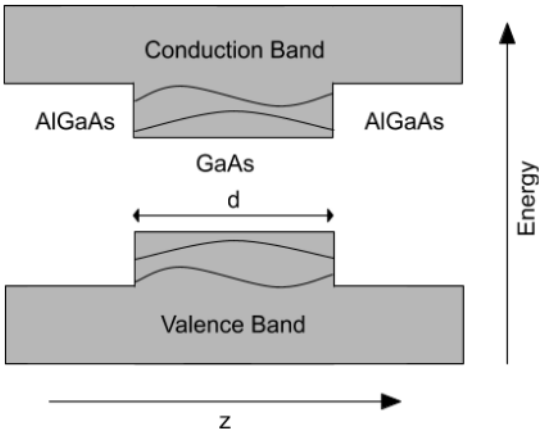
Introduction

A Quantum Well is essentially a potential well that has discrete energy levels. Quantum Wells are double heterostructures i.e. when two semiconductor materials are grown simultaneously into a sandwich.



One very famous example of a double heterostructure that is an excellent example for study of Quantum Well Structures is AlGaAs – GaAS. For purpose of this report, we shall stick to data of this structure for purpose of understanding the theory and logic of these programs. However the program is designed keeping in mind all the basic physics of quantum well structures.

Quantum Confinement

One important effect that is observed in quantum well structures is the effect of quantum confinement. Quantum Confinement is restriction on free flow motion of electrons or holes in one or more directions. Based on degree of freedom of electrons, we classify type of semiconductors as follows

- 3D : Bulk Semiconductors (No confinement)
- 2D : Quantum Wells (Confinement in 1 direction)
- 1D : Quantum Wired (Confinement in 2 direction)
- 0D : Quantum Dots (Confinement in 3 directions)

In our project, we simulate Quantum Wells. Quantum Confinement effects is observed when one dimension of well reaches quantum size i.e., the dimensions of well are comparable to that of De-Broglie wavelength of electron in the material. The physics of Quantum Well is very similar to finite potential model of quantum mechanics.

Finite Potential Well

The finite square well, defined as follows and shown in figure,

$$V(x) = \begin{cases} -V_0\,, & \text{for} \quad |x| \leq a\,, \quad V_0 > 0\,, \\ 0\,, & \text{for} \quad |x| \geq a\,. \end{cases}$$

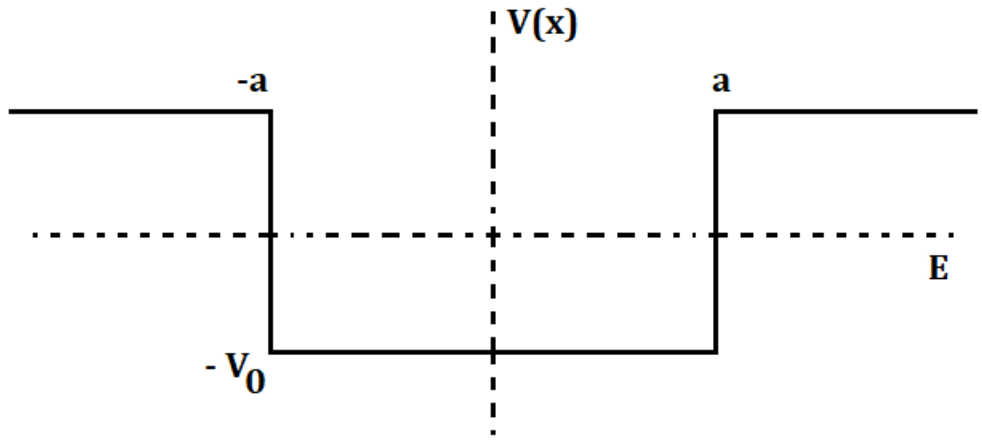


Figure 1: The finite potential well

Note that the potential energy is zero for x > a. The potential energy is negative and equal to $-V_0$ in the well, because we defined V_0 to be a positive number. The width of the well is 2a. Note also that we have placed the bottom of the well differently than in the case of the infinite square well. The bottom of the infinite square well was at zero potential energy. If we wanted to obtain the infinite square well as a limit of the finite square well we would have to take V_0 to infinity, but care is needed to compare energies. The ones in the infinite square well are measured with respect to a bottom at zero energy. The ones in the finite square well are measure with respect to a bottom at $-V_0$.

We will be interested in **bound states** namely, energy eigenstates that are normalizable. For this the energy E of the states must be negative. This is readily understood. If E > 0, any solutions in the region x>a where the potential vanishes would be a plane wave, extending all the way to infinity. Such a solution would not be normalizable. The energy E is shown as a dashed line in the figure. We have

$$-V_0 < E < 0$$

Note that since E is negative we have $\mathrm{E} = -\,|\,E\,|$. For a bound state of energy E, the energy E measured with respect to the bottom of the potential is

$$\overline{E} = E - (-V_0) = V_0 - |\,E\,| > 0$$

Those $\overline{E}$ are the ones that can be compared with the energies of the infinite square well in the limit as $V \longrightarrow \infty$.

What are the bound state solutions to the Schrodinger equation with this potential? We have to examine how the equation looks in the various regions where the potential is constant

and then use boundary conditions to match the solutions across the points where the potential is discontinuous. We have the equation Let's examine the regions, where, for simplicity, we define A(x) by

$$\frac{d^2\psi}{dx^2} = -\frac{2m}{\hbar^2}(E - V(x))\,\psi = \alpha(x)\psi\,,$$

where we have defined the factor $\alpha(x)$ that multiplies the wavefunction on the right hand side of the Schrodinger equation. We then consider the two regions

- region $\mid x \mid > a$: $\alpha(x)$ is a positive constant. The wavefunction in this region constructed with real exponentials.
- region $\mid x \mid < a$: $\alpha(x)$ is a negative constant. The wavefunction in this region is constructed with trigonometric functions.

The potential V(x) for the finite square well is an even function of $x : V(-x) = V(x)$ We can therefore use the theorem cited earlier that for an even potential the bound states are either symmetric or anti-symmetric. We begin by looking for even solutions, that is, solutions ψ for which $\psi(-x) = \psi(x)$.

Even solutions : Since the potential is piecewise continuous we must study the differential equation in two regions:

- $|x| < a$

$$\frac{d^2\psi}{dx^2} = -\frac{2m}{\hbar^2}(E - (-V_0))\psi = -\frac{2m}{\hbar^2}(V_0 - |E|)\psi$$

$V_0 - |E|$ is a positive constant thus define a real $k > 0$ by

$$\boxed{k^2 \equiv \frac{2m}{\hbar^2}(V_0 - |E|) > 0\,, \quad k > 0\,.}$$

It is interesting to note that this equation is not too different from the free-particle equation $k^2 = \frac{2mE}{\hbar^2}$. Indeed, $V_0 - |E|$ is the kinetic energy of the particle and thus k has the usual interpretation. The differential equation to be solved now reads

$$\psi'' = -k^2\psi\,,$$

for which the only possible even solution is

$$\boxed{\psi(x) = \cos kx\,, \quad |x| < a\,.}$$

We are not including a normalization constant because, at this state we do not aim for normalized eigenstates. We will get an eigenstate and while it will not be normalized, it will be *normalizable*, and that's all that is essential. We are after is the possible energies. Normalized wavefunctions would be useful to compute expectation values.

- $|x| > a$

$$\psi'' = -\frac{2m}{\hbar^2}(E-0)\,\psi = \frac{2m|E|}{\hbar^2}\,\psi$$

This time we define a real positive constant κ with the relation

$$\boxed{\kappa^2 = \frac{2m|E|}{\hbar^2}, \quad \kappa > 0\,.}$$

The differential equation to be solved now reads

$$\psi'' = \kappa^2\psi\,,$$

and the solutions are exponentials. In fact we need exponentials that decay as $x \to \pm\infty$, otherwise the wavefunction will not be normalizable. This should be physically intuitive, in a classically forbidden region the probability to be far away from the well must be vanishingly small. For $x > a$ we choose the decaying exponential

$$\boxed{\psi(x) = A\,e^{-\kappa x}, \;\; x > a\,,}$$

where A is a normalization constant to be determined by the boundary conditions. More generally, given that the solution is even, we have

$$\psi(x) = A\,e^{-\kappa|x|}, \; |x| > a\,.$$

It is now useful to note that κ^2 and k^2 satisfy a simple relation. Using their definition above we see that the energy $|\,E\,|$ drops out of their sum and we have

$$k^2 + \kappa^2 = \frac{2mV_0}{\hbar^2}$$

At this point we make progress by introducing unit free constants $\xi, \eta, and z_0$ as follows:

$$\begin{aligned}
\eta &\equiv ka > 0\,,\\
\xi &\equiv \kappa a > 0\,,\\
z_0^2 &\equiv \frac{2mV_0a^2}{\hbar^2}\,.
\end{aligned}$$

Clearly ξ is a proxy for κ and η is a proxy for k. Both depend on the energy of the bound state. The parameter z_0, unit-free, just depends on the data associated with the potential (the depth V_0 and the width 2a) and the mass m of the particle. If you are given a potential, you know the number z_0. A very deep and/or wide potential has very large z_0, while a very shallow and/or narrow potential has small z_0. As we will see the value of z_0 tells us how many bound states the square well has.
Multiplying the "circle equation" by a^2 and using our definitions above we get

$$\boxed{\eta^2 + \xi^2 \;=\; z_0^2 \,.}$$

Let us make clear that solving for ξ is actually like solving for the energy.

$$\xi^2 \;=\; \kappa^2 a^2 \;=\; \frac{2m|E|a^2}{\hbar^2} \;=\; \frac{2mV_0a^2}{\hbar^2}\frac{|E|}{V_0} \;=\; z_0^2\frac{|E|}{V_0}\,,$$

and from this we get

$$\frac{|E|}{V_0} = \Big(\frac{\xi}{z_0}\Big)^2 .$$

This is a nice equation, the left hand side gives the energy as a fraction of the depth V_0 of the well and the right hand side involves ξ and the constant z_0 of the potential. The quantity η also encodes the energy in a slightly different way. from relation of k and E,V we have

$$\eta^2 \;=\; k^2a^2 \;\equiv\; \frac{2ma^2}{\hbar^2}(V_0 - |E|)\,,$$

Let us finally complete the construction. We must impose the continuity of the wavefunction and the continuity of ψ' at x = a. Using the expressions for ψ for x < a and for x > a these conditions give

$$\begin{aligned} \psi \text{ continuous at } x=a \implies \quad \cos(ka) &= Ae^{-\kappa a} \\ \psi' \text{ continuous at } x=a \implies \quad -k\sin(ka) &= -\kappa Ae^{-\kappa a}\,, \end{aligned}$$

Dividing the second equation by the first we eliminate the constant A and find a second relation between k and κ! This is exactly what is needed. The result is

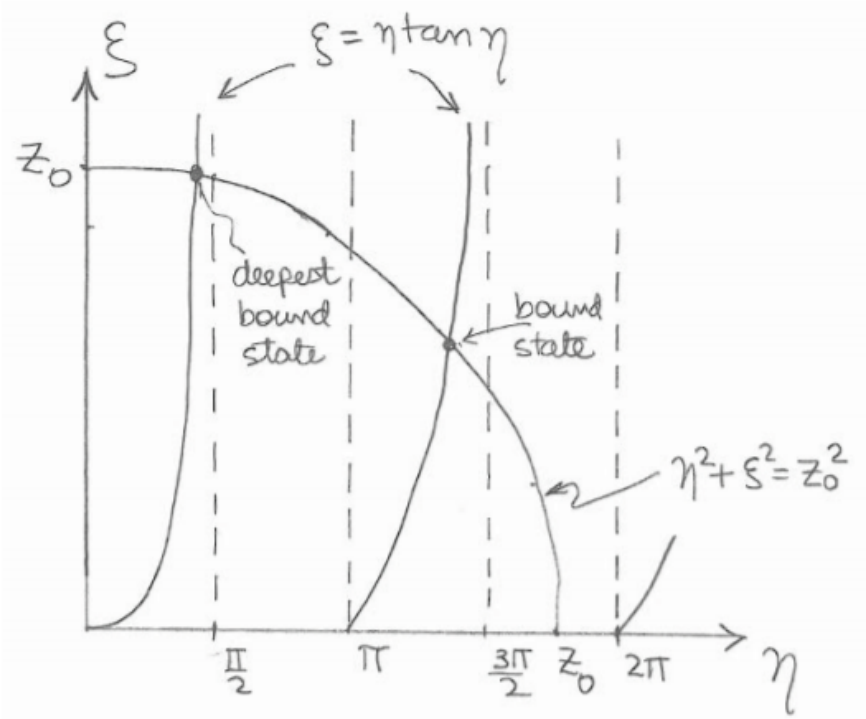
$$k\tan ka \;=\kappa \quad\to\quad ka\tan ka \;=\kappa a \quad\to\quad \xi = \eta\tan\eta\,. \tag{2.33}$$

Our task of finding the bound states is now reduced to finding solutions to the simultaneous equations

$$\boxed{\text{Even solutions: } \eta^2+\xi^2 \;=\; z_0^2\,, \quad \xi = \eta\tan\eta\,, \quad \xi\,,\eta > 0\,.} \tag{2.34}$$

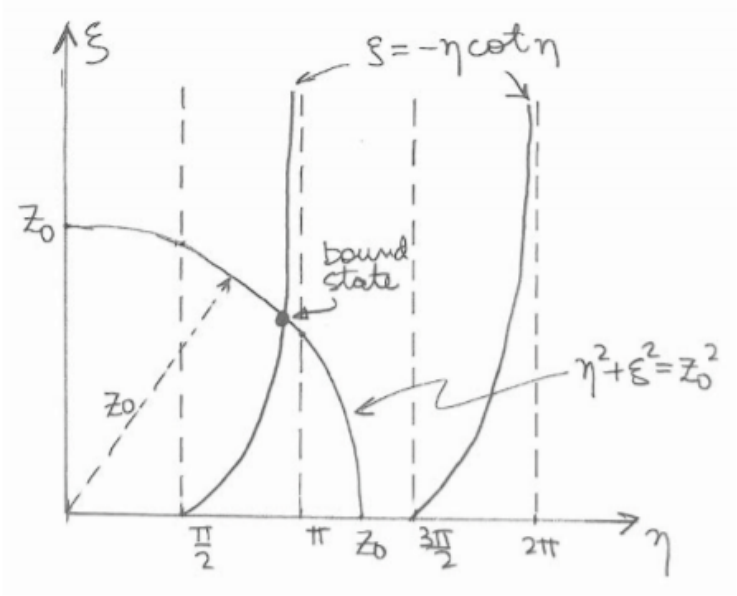
These equations can be solved numerically to find all solutions that exist for a given fixed value of z_0. Each solution represents one bound state. We can understand the solution space

by plotting these two equations in the first quadrant of an (η, ξ) plane, as shown in next figure.



The first equation of even solution is a piece of a circle of radius z_0. The second equation, $\xi = \eta tan\eta$, gives infinitely many curves as η grows from zero to infinity. The value of ξ goes to infinity for η approaches each odd multiple of $\pi/2$. The bound states are represented by the intersections in the plot (heavy dots).

In the figure we see two intersections, which means two bound states. The first intersection takes place near $\eta = \pi/2$ and with large $\eta \sim z_0$. This is the ground state, or the most deeply bound bound-state. Alternatively, noting that this is the solution with smallest η. The second solution occurs for η near $3\pi/2$. As the radius of the circle becomes bigger we get more and more intersections; z_0 controls the number of even bound states. Finally, note that there is always an even solution, no matter how small z_0 is, because the arc of the circle will always intersect the first curve of the $\xi = \eta tan\eta$ plot. Thus, at least one bound state exists however shallow the finite well is.



Odd solutions. For odd solutions all of our definitions $(k, \kappa, z_0, \eta, \xi)$ remain the same. The wavefunction now is of the form

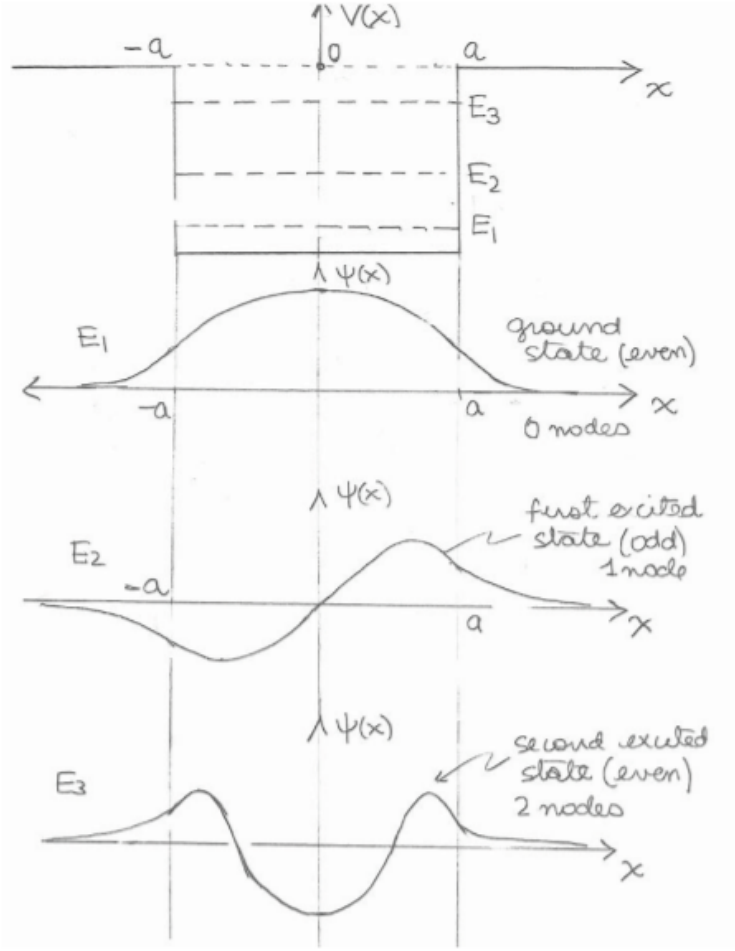
$$\psi(x) = \begin{cases} \sin kx\,, & |x| < a \\ Ae^{-k|x|}\,, & |x| > a \end{cases}$$

Matching ψ and ψ' at $x = a$ now gives $\xi = -\eta \cot \eta$ (do it!). As a result the relevant simultaneous equations are now

$$\boxed{\text{Odd solutions:} \quad \eta^2 + \xi^2 = z_0^2\,, \quad \xi = -\eta \cot \eta\,, \quad \xi\,, \eta > 0\,.}$$

In the above figure the curve $\xi = -\eta cot\eta$ does not appear for $\eta < \pi/2$ because ξ is then negative. For $z_0 < \pi/2$ there are no odd bound-state solutions, but we still have the even bound state.

We could have anticipated the quantization of the energy by the following argument. Suppose you try to calculate energy eigenstates which, as far as solving the Schrodinger equation, are determined up to an overall normalization. Suppose you don't know the energy is quantized and you fix some arbitrary fixed energy and calculate. Both in the even and in the odd case, we can set the coefficient of the sin(kx) or cos(kx) function inside the well equal to one. The coefficient of the decaying exponential outside the well was undetermined, we called it A. Therefore we just have one unknown, A. But we have two equations, because we impose continuity of ψ and of ψ_0 at x = a. If we have one unknown and two equations, we have no reason to believe there is a solution. Indeed, generally there is none. But then, if we think of the energy E as an unknown, that energy appears at various places in the equations (in k and κ) and therefore having two unknowns A and E and two equations, we should expect a single solution This is indeed what happened.



In the figure above we sketch the energy eigenstates of a square-well potential with three bound states of energies $E_1 < E_2 < E_3$. A few features of the wavefunctions are manifest: they alternate as even, odd, and even. They have zero, one, and two nodes, respectively. The second derivative of ψ is negative for x < a and positive for x > a (it is in fact discontinuous at x = ±a). The exponential decay in the region x > a is fastest for the ground state and slowest for the least bound state.

Photonics of Quantum Well

Important result from finite potential model solution are

- Energy in Quantum Wells are discreticised
- Lower the width of Well, more discreticised are the energy levels
- Wave vector number k is discreticied and is inversely proportional to width of well.

As the width of well is decreased, effective bandgap of "Low Band Gap" materials increases. The difference in bandgaps of Low Band Gap materials and High Band Gap materials is what forms a well with barriers of high band gap materials on either side, confining the electrons and

holes.

Any electron lying in valence band of Active region (low band gap material) can absorb a photon of energy $h\nu \geq E_g(eff)$ and jump to conduction band. This transitions have a certain set of rules. An electron in n=1 valence band can only jump to n=1 conduction band energy level. Similarly, An electron in n=2 valence band can only jump to n=2 conduction band energy level and so on.

Probabilistically, n=1 transitions are the most favourable. Throughout this program we have only considered n=1 transition.

An electron in conduction band can recombine with hole in valence band, emitting a photon in process. The energy of photon is equal to energy difference between energy level in conduction band and valence band. For n=1, the effective bandgap of active region is given by

$$E_g(eff) = E_g(active) + \frac{\hbar^2 k^2}{2M_{eff}} \tag{1}$$

Here,

- $E_g(active)$ = Bandgap energy of Low Bandgap Material
- $M_{eff} = \frac{1}{M_e} + \frac{1}{M_h}$

where
M_e = effective mass of electrons in Low Bandgap Material
M_h = effective mass of holes in Low Bandgap Material
k = $\frac{\pi}{L}$ is the wavenumber and L is width of well

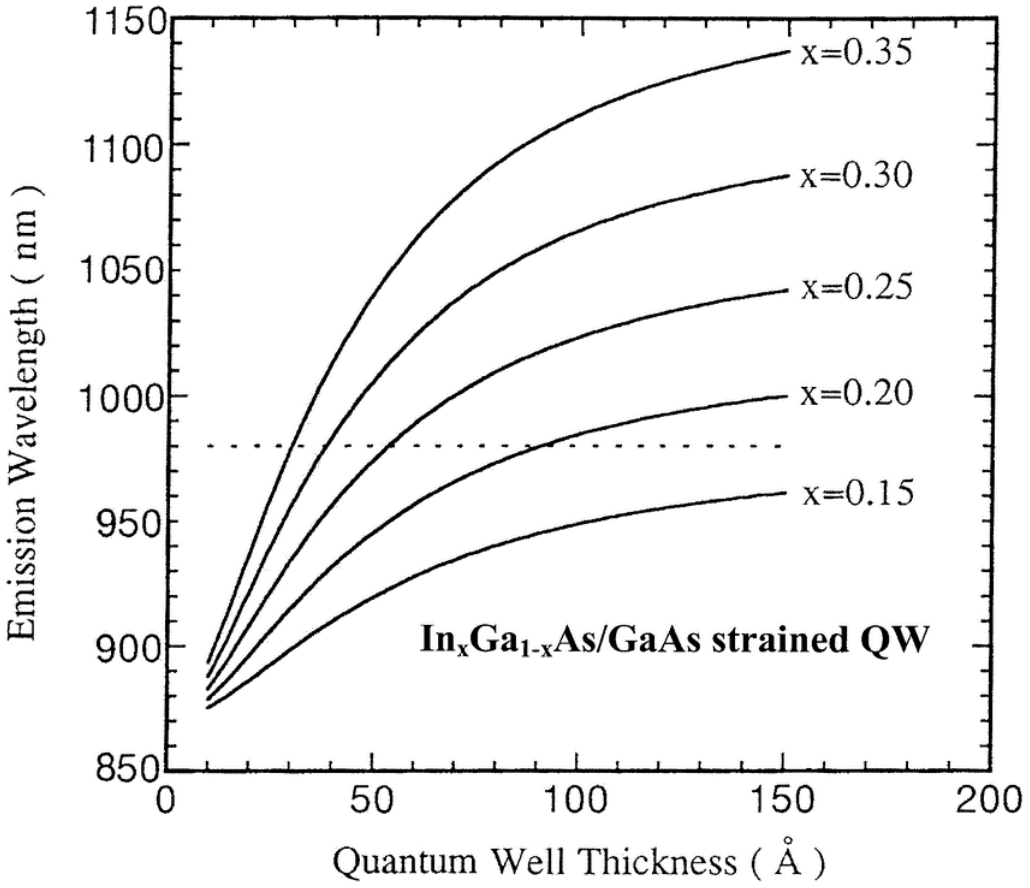
From equation (1), we see that larger the value of k (lower the width of well), higher is the effective bandgap of material.

Now,

$$\frac{hc}{\lambda} = E_g(eff) \tag{2}$$

$$\lambda(\mu m) = \frac{1.23}{E_g(eff)} \tag{3}$$

From equation (1) and (3), the relation between emission wavelength and width of quantum well is evident.

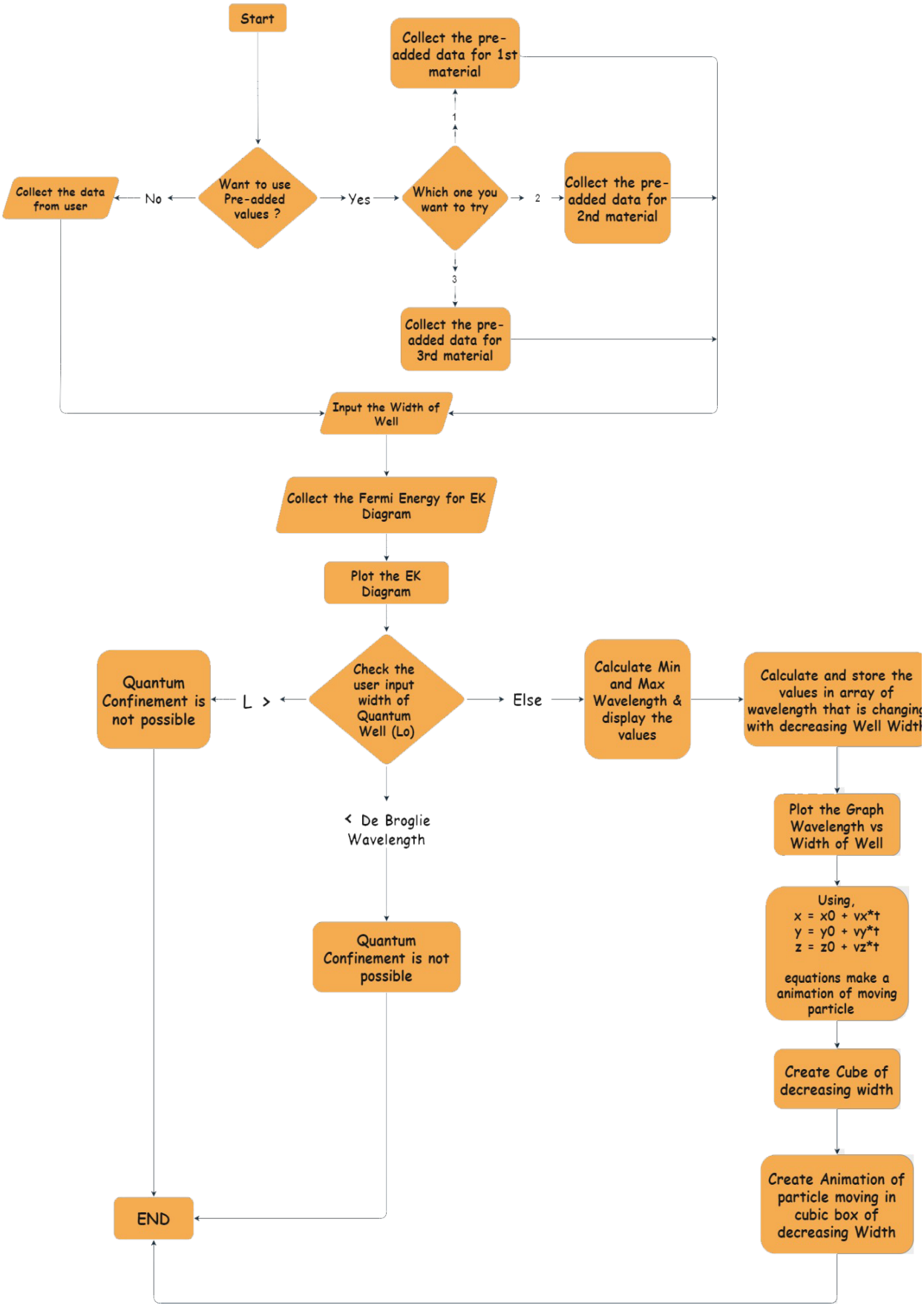


Program Description

User Input

- Bandgap of Low gap and High Gap material (in eV)
- Effective mass of electrons and holes (Light Holes and Heavy Holes) of Low Gap material (in fraction form i.e., $x \cdot M_0$, $M_0 = 9.31 \times 10^{-31}$ kg)
- Fermi conduction and valence level of Low Gap material (in eV)
- Width of quantum well (in nm)
- Thermal velocity of electron in Low Gap Layer (in m/s)

Flow Chart


Start
Collect the pre-added data for 1st material
1
Want to use Pre-added values ?
No
Collect the data from user
Yes
Which one you want to try
2
Collect the pre-added data for 2nd material
3
Collect the pre-added data for 3rd material
Input the Width of Well
Collect the Fermi Energy for EK Diagram
Plot the EK Diagram
Check the user input width of Quantum Well (Lo)
L >
Quantum Confinement is not possible
Else
Calculate Min and Max Wavelength & display the values
Calculate and store the values in array of wavelength that is changing with decreasing Well Width
< De Broglie Wavelength
Quantum Confinement is not possible
Plot the Graph Wavelength vs Width of Well
Using,
x = x0 + vx*t
y = y0 + vy*t
z = z0 + vz*t
equations make a animation of moving particle
Create Cube of decreasing width
Create Animation of particle moving in cubic box of decreasing Width
END

Results in Output

- Emission Wavelength for given width of well (in nm)
- Minimum possible Emitted Wavelength (in nm)
- Maximum possible emitted Wavelength (in nm)
- Minimum Width of Well required to observe quantum confinement effect based on user input material data (in nm)
- De-Broglie Wavelength of electron based on user input material data
- Emission Wavelength vs Width of Well graph
- Energy vs Wavevector (EK diagram) of low gap material
- Animation that shows how electron is moving in Quantum Well of decreasing length.

Code

```
clc;
clear all;
#-----------------------------------------------------------------------
#                      Simulation of Quantum Confinement
#-----------------------------------------------------------------------
#-----------------------------------------------------------------------
#                                  Instructions
#-----------------------------------------------------------------------
disp("-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.--.-.-.-.-.-.")
disp("           WELCOME TO THE SIMULATION OF QUANTUM CONFINEMENT    ")
disp("-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.--.-.-.-.-.-.")
disp("Here are some examples of Quantum Well Structure if you want to
try ...  ")
disp(" ")
disp("1) GaAs & AlGaAs")
disp("  # Active Material : GaAs ")
disp("  # Cladding Material : AlGaAs ")
disp("  # Bandgap of Active Region : 1.42 eV ")
disp("  # Bandgap of Cladding Region : 1.80 eV ")
disp("  # Effective Mass of Electron : 0.063 ")
disp("  # Effective Mass of Light Hole : 0.082 ")
disp("  # Effective Mass of Heavy Hole : 0.54 ")
disp("  # Thermal Velocity of Electron : 4.4 * 10^5 m/s ")
disp(" ")
disp("2) GaInAs & InP ")
disp("  # Active Material : GaInAs ")
disp("  # Cladding Material :  InP ")
disp("  # Bandgap of Active Region : 0.75 eV ")
disp("  # Bandgap of Cladding Region : 1.35 eV ")
disp("  # Effective Mass of Electron : 0.041 ")
disp("  # Effective Mass of Light Hole : 0.051 ")
disp("  # Effective Mass of Heavy Hole : 0.47 ")
disp("  # Thermal Velocity of Electron : 5.5 * 10^5 m/s ")
disp(" ")
disp("3) InGaAs & GaAs ")
disp("  # Active Material : InGaAs ")
disp("  # Cladding Material : GaAs ")
disp("  # Bandgap of Active Region : 0.75 eV ")
disp("  # Bandgap of Cladding Region : 1.42 eV ")
disp("  # Effective Mass of Electron : 0.041 ")
disp("  # Effective Mass of Light Hole : 0.082 ")
disp("  # Effective Mass of Heavy Hole : 0.54 ")
disp("  # Thermal Velocity of Electron : 5.5 * 10^5 m/s ")
disp(" ")
disp("-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.--.-.-.-.-.-.")
disp(" ")
disp(" ")
disp("................................................................")
#-----------------------------------------------------------------------
#                 Want to try from above or your own material
#-----------------------------------------------------------------------
```

```
option1 = input("Do you want to try for one of the above Materials ??
(1 = Yes, 0 = No) : ");

# Want to try from above material
if option1==1
  yes = input("Enter the number 1,2 or 3 : ");

  # 1st material
  if yes==1
    disp("You chose the material : GaAs/AlGaAs ")

disp("............................................................")
    Eg = 1.42;
    Eg2 = 1.80;
    Me = 0.063;
    Ml = 0.082;
    Mh = 0.54;
    V = 4.4*10^5;

  # 2nd material
  elseif yes==2
    disp("You chose the material : GaInAs/InP ")

disp("............................................................")
    Eg = 0.75;
    Eg2 = 1.35;
    Me = 0.041;
    Ml = 0.051;
    Mh = 0.47;
    V = 5.5*10^5;

  # 3rd Material
  elseif yes==3
    disp("You chose the material : GaAs/InGaAs ")

disp("............................................................")
    Eg = 0.75;
    Eg2 = 1.42;
    Me = 0.041;
    Ml = 0.082;
    Mh = 0.54;
    V = 5.5*10^5;

  # Incorrect Value
  else
    disp("Please Enter Correct Value")
    return
  endif
  Lo = input("Please enter width of Quantum Well(in nm) : ");

# Want to try your own material
elseif option1==0
disp("............................................................")
disp("                Input the Values for your own material          ")
disp("............................................................")
```

```
Eg = input("Please enter bandgap of active region in eV : ");
Eg2 = input ("Bandgap of cladding material in eV : ");
Me = input("Effective mass of electron in 'x*M0' form : ");
Ml = input("Effective mass of light holes in 'x*M0' form : ");
Mh = input("Effective mass of heavy holes in 'x*M0' form : ");
V = input("Thermal velocity of electrons : ");
Lo = input("Please enter width of Quantum Well(in nm) : ");

# Incorrect Value
else
disp("Please Enter Correct Value")
return

endif
# Average effective mass of holes
Mv = ((Ml)^1.5 + (Mh)^1.5)^(2/3);

L = (0.6069/(sqrt(Eg2 - Eg)))*sqrt(1/Me + 1/Ml);
disp("..........................................................")
display("For EK Diagram")
disp(" ")
Efc = input("Please Enter Fermi Conduction Bandgap of Material in eV :
");
Efv = input("Please Enter Fermi Valence Bandgap of Material in eV : ");
disp("..........................................................")


#-------------------------------------------------------------------
#                          EK Diagram for Active Region
#-------------------------------------------------------------------
Evm = []; # Valence Bandgap Energy Array
Ecm = []; # Conduction Bandgap Energy Array
Ev1m = []; # Light Hole Valence Bandgap Energy Array
Ev2m = []; # Heavy Hole Valence Bandgap Energy Array
Km = []; # Wave-vector Array
h = 1*10^(-34); # Reduced Plank Constant
n = -10;
for i=1:1:21
  n++;
  K = n*pi/(Lo*10^(-9)); # Wave Vector

  Ev1 = Efv - ((h^2)*(K^2))/(2*Ml*9.31*10^(-31)*1.6*10^(-19)); # Energy
of light holes Valence Band
  Ev2 = Efv - ((h^2)*(K^2))/(2*Mh*9.31*10^(-31)*1.6*10^(-19)); # Energy
of heavy holes Valence Band
  Ev = Efv - ((h^2)*(K^2))/(2*Mv*9.31*10^(-31)*1.6*10^(-19)); # Energy
of Valence Band
  Ec = Efc + ((h^2)*(K^2))/(2*Me*9.31*10^(-31)*1.6*10^(-19)); # Energy
of Conduction Band
  Evm(i) = Ev; # Store the data in array
  Ecm(i) = Ec; # Store the data in array
  Ev1m(i) = Ev1; # Store the data in array
  Ev2m(i) = Ev2; # Store the data in array
  Km(i) = K; # Store the data in array
  i++;
```

```
end
#-------------------------------------------------------------------------
#                              Figure (1) : EK Diagram
#-------------------------------------------------------------------------
figure(1)

  plot(Km,Evm,"linewidth",3,'m');
  hold on;
  plot(Km,Ecm,"linewidth",3,'k');
  hold on
  plot(Km,Ev1m,"linewidth",3,'--y');
  hold on;
  plot(Km,Ev2m,"linewidth",3,'--g');
  hold on

legend("Valence Band (Average Effective Mass of Holes)","Conduction
Band","Valence Band (Light Holes)","Valence Band (Heavy Holes)",
       "location","south")

  str1=sprintf("Bandgap E_g = %d eV \n",Efc-Efv);

text(0,(Efc+Efv)/2,{str1},"horizontalalignment","center",'FontSize',15,
'Color',[0.2,0.4,1],'FontWeight','bold')
  str2=sprintf(" ");
  str3=sprintf("E-K Diagram for Active Material");
  set(gca,"linewidth",2,"fontsize",12,'FontWeight','bold')

title({str2,str3,str2},'FontSize',20,'Color',[0,0,0],'FontWeight','bold
')

  xlabel("Wave Vector k
(m)",'FontSize',13,'Color','k','FontWeight','bold')
  ylabel("Energy E (eV)",'FontSize',13,'Color','k','FontWeight','bold')

  axis("square")



#-------------------------------------------------------------------------
#              Check Whether Quantum Confinement is Possible or not
#-------------------------------------------------------------------------
Lamda_D = 6.63*10^(-25)/(Me*V*9.31*10^(-31));
# Condition : 1 when quantum confinement will not observe
if ( Lo > Lamda_D)
  Lamda_E = 1.23*1000/Eg ; # Maximum Wavelength that can be emitted
  printf("Emission Wavelenth = %d \n",Lamda_E);
  printf("\n Effects of Quantum Confinement not observed. \n");
  printf("\n Width of Quantum Well should be equal to or less than De-
Broglie Wavelength of Electron \n");
  printf("\n De-Broglie Wavelength of electron is = %d \n",Lamda_D);
  return;

# Condition : 2 when quantum confinement will not observe
elseif ( Lo < L)
```

```
  printf("For given material at %d nm (Quantum Well Width), Length of
well exceeds minimum practical length \n",Lo)
  printf("Please enter length of well that exceeds > %d nm\n",L)
  return;

# Condition : 3 when quantum confinement will observe
else
  Lamda_E = 1.23*1000/(Eg + (0.369/Lo^2)*(1/Me + 1/Mv)); # Emission
Wavelenght
  display("\n Here are your results");
  printf("\n # Emission Wavelenth = %d nm\n",Lamda_E);
endif

Lamda_max = 1.23*1000/Eg; # Maximum Emission Wavelength
Lamda_Min = 1.23*1000/Eg2; # Minimum Emission Wavelength

printf("\n # Practical Minimum Emission Wavelenth = %d
nm\n",Lamda_Min);
printf("\n # Practical Maximum Emission Wavelenth = %d
nm\n",Lamda_max);
printf("\n # Minimum optimum well width = %d nm\n",L);
printf("\n # Maximum well width upto which Quantum Confinment can be
observed = %d nm\n",Lamda_D);
disp("...............................................................")

#-------------------------------------------------------------------
#      Calculation of Wavelength as a function of Decreasing Well Width
#-------------------------------------------------------------------
Lamda_E1_matrix = []; # Emission Wavelength Array
Lm=[]; # Width of Well Array
counter=1; # Counter

for i = L:0.08:Lo
  Lm(counter)=i;
  Lamda_E1 = 1.23*1000/(Eg + (0.369/i^2)*(1/Me + 1/Mv)); # Emission
Wavelength with Decreasing Width

  # If wavelength will be higher than the maximum it will become
constant to it max value
  if Lamda_E1>Lamda_max
    Lamda_E1=Lamda_max;

  # If wavelength will be lower than the minimum it will become
constant to it min value
  elseif Lamda_E1<Lamda_Min
    Lamda_E1=Lamda_Min;

  endif

  Lamda_E1_matrix(counter) = Lamda_E1; # Store the wavelength value in
array
  counter+=1;
end
#-------------------------------------------------------------------
#             Figure (2) :  Wavelength vs Width of Well Graph
```

```
#-----------------------------------------------------------------------
figure(2)

plot(Lm,Lamda_E1_matrix,'r',"linewidth",3);

ylabel("Emission Wavelength
(nm)",'FontSize',13,'Color','k','FontWeight','bold');
xlabel("Length of Well
(nm)",'FontSize',13,'Color','k','FontWeight','bold');

str2=sprintf(" ");
str3=sprintf("Wavelength vs Width of Well");
set(gca,"linewidth",2,"fontsize",12,'FontWeight','bold')
title({str2,str3,str2},'FontSize',20,'Color',[0,0,0],'FontWeight','bold
')

axis("square")



#-----------------------------------------------------------------------
#                       Calculations to create Animation
#-----------------------------------------------------------------------
v=20; # Initial Velocity of particle

theta_d = 23; # Initial angle of particle in xy direction
theta=theta_d*pi/180; # Convert theta in radian

phi_d = 23; # Initial angle of particle in z direction
phi=phi_d*pi/180; # Convert theta in radian

vx=v*cos(theta)*sin(phi); # Calculate x component of velocity
vy=v*sin(theta)*sin(phi); # Calculate y component of velocity
vz=v*cos(phi); # Calculate z component of velocity

x=2; # Initial x coordinate of particle
y=3; # Initial y coordinate of particle
z=1; # Initial z coordinate of particle

a = 30; # Acceleration



#-----------------------------------------------------------------------
#Figure (3): Animation How Electron moves in Quantum Well of Decreasing
Width
#-----------------------------------------------------------------------
figure(3)

# Calculations for moving particle
for i=1:counter-1

x = x + vx*0.1;
y = y + vy*0.1;
z = z + vz*0.1;
```

```
vx = vx + a*0.1;
vy = vy + a*0.1;
vz = vz + a*0.1;

if x<0
  x=0;
  vx=-vx;

elseif x>=Lm(counter-i)
  x = Lm(counter-i);
  vx = -vx;

endif


if y<0
  y = 0;
  vy = -vy;

elseif y>=Lo
  y = Lo;
  vy = -vy;

endif


if z<0
  z = 0;
  vz = -vz;

elseif z>=Lo
  z = Lo;
  vz = -vz;

endif

# Creating 3D Box of decrasing width
line_0toLo = linspace(0,Lo,counter-1);
line_xyz0 = zeros(1,counter-1);
line_fixLo = Lo*ones(1,counter-1);

plot3(line_xyz0,line_xyz0,line_0toLo,'k','linewidth',5);
hold on
plot3(line_xyz0,line_fixLo,line_0toLo,'k','linewidth',5);
hold on
plot3(line_xyz0,line_0toLo,line_fixLo,'k','linewidth',5);
hold on

q=quiver3(0,0,Lo,Lm(counter-
i),0,0,'k','linewidth',5,'ShowArrowHead','off');
r=quiver3(0,Lo,Lo,Lm(counter-
i),0,0,'k','linewidth',5,'ShowArrowHead','off');
```

```
s=quiver3(Lm(counter-
i),0,0,0,0,Lo,'k','linewidth',5,'ShowArrowHead','off');
t=quiver3(Lm(counter-
i),Lo,0,0,0,Lo,'k','linewidth',5,'ShowArrowHead','off');
u=quiver3(Lm(counter-
i),0,Lo,0,Lo,0,'k','linewidth',5,'ShowArrowHead','off');

b=rectangle('Position',[0 0 Lm(counter-i) Lo],'linewidth',5);
hold on
c=plot3(x,y,z,'.r','markersize',50);



str2=sprintf(" ");
str3=sprintf("Electron moving in Quantum Well of Decreasing Width");
set(gca,"linewidth",2,"fontsize",12,'FontWeight','bold')
title({str2,str3,str2},'FontSize',20,'Color',[0,0,0],'FontWeight','bold
')

xlabel("Width of Quantum
Well",'FontSize',13,'Color','k','FontWeight','bold')
axis([0 Lo 0 Lo 0 Lo],"square")

pause(0.01)

if i<(counter-1)
  delete(c)
  delete(b)
  delete(q)
  delete(r)
  delete(s)
  delete(t)
  delete(u)
endif

end

#-------------------------------------------------------------------------
#                                   END OF PROGRAM
#-------------------------------------------------------------------------
```

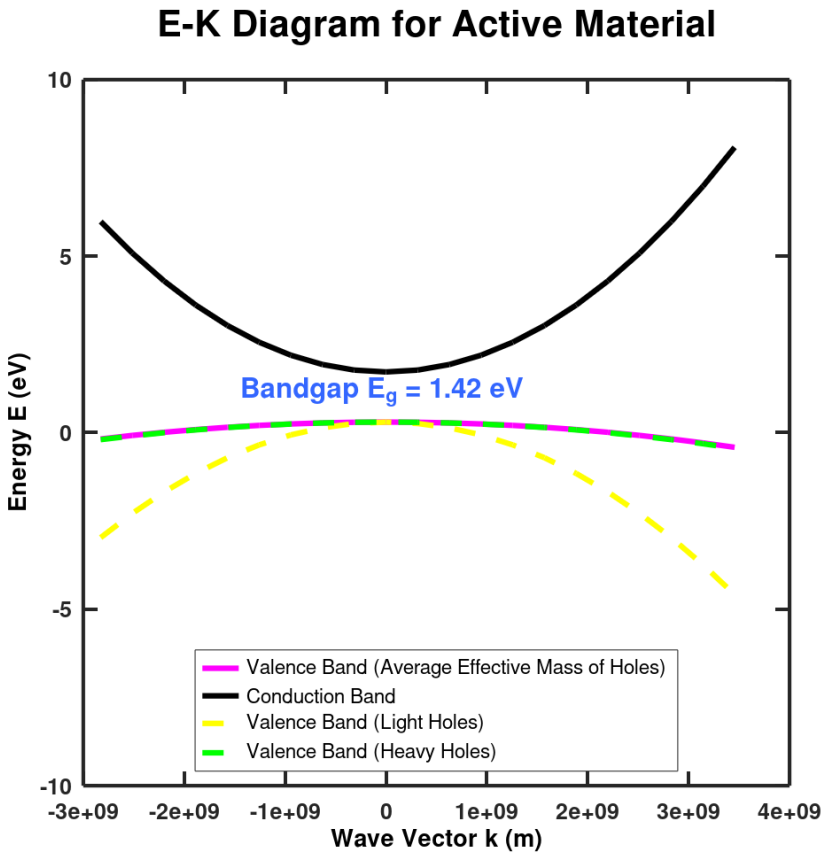
Output :

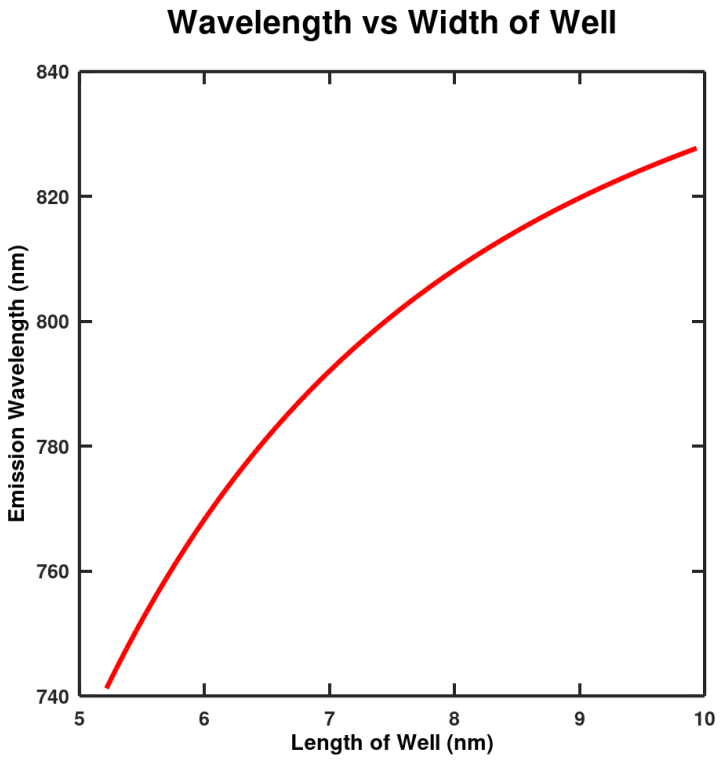
- **Command Window**

```
-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.--.-.-.-.-.-.-.-.-.-.-.-.
           WELCOME TO THE SIMULATION OF QUANTUM CONFINEMENT
-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.--.-.-.-.-.-.-.-.-.-.-.-.
Here are some examples of Quantum Well Structure if you want to try ...

1) GaAs & AlGaAs
  # Active Material : GaAs
  # Cladding Material : AlGaAs
  # Bandgap of Active Region : 1.42 eV
  # Bandgap of Cladding Region : 1.80 eV
  # Effective Mass of Electron : 0.063
  # Effective Mass of Light Hole : 0.082
  # Effective Mass of Heavy Hole : 0.54
  # Thermal Velocity of Electron : 4.4 * 10^5 m/s

2) GaInAs & InP
  # Active Material : GaInAs
  # Cladding Material :  InP
  # Bandgap of Active Region : 0.75 eV
  # Bandgap of Cladding Region : 1.35 eV
  # Effective Mass of Electron : 0.041
  # Effective Mass of Light Hole : 0.051
  # Effective Mass of Heavy Hole : 0.47
  # Thermal Velocity of Electron : 5.5 * 10^5 m/s

3) InGaAs & GaAs
  # Active Material : InGaAs
  # Cladding Material : GaAs
  # Bandgap of Active Region : 0.75 eV
  # Bandgap of Cladding Region : 1.42 eV
  # Effective Mass of Electron : 0.041
  # Effective Mass of Light Hole : 0.082
  # Effective Mass of Heavy Hole : 0.54
  # Thermal Velocity of Electron : 5.5 * 10^5 m/s

-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.-.--.-.-.-.-.-.-.-.-.-.-.-.
```

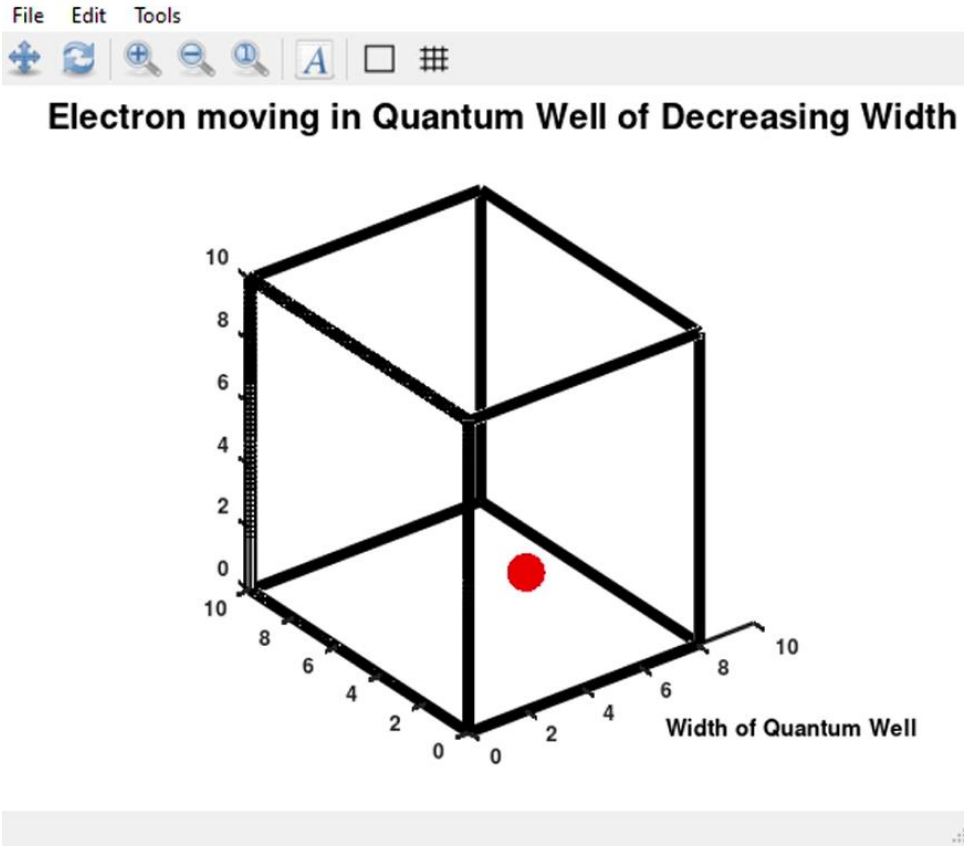
```
.....................................................................
Do you want to try for one of the above Materials ?? (1 = Yes, 0 = No) : 1
Enter the number 1,2 or 3 : 1
You chose the material : GaAs/AlGaAs
.....................................................................
Please enter width of Quantum Well(in nm) : 10
.....................................................................
For EK Diagram

Please Enter Fermi Conduction Bandgap of Material in eV : 1.72
Please Enter Fermi Valence Bandgap of Material in eV : 0.30
.....................................................................

 Here are your results

 # Emission Wavelenth = 828.2 nm

 # Practical Minimum Emission Wavelenth = 683.333 nm

 # Practical Maximum Emission Wavelenth = 866.197 nm

 # Minimum optimum well width = 5.21593 nm

 # Maximum well width upto which Quantum Confinment can be observed = 25.6904 nm
.....................................................................
```

- Output





- Animation File : Click Here



Applications of Quantum Well

Quantum well systems can be used to create compact, fast computer chips, highly efficient microscopic lasers, and optoelectronic devices; they form the basis of lasers in CD players and microwave receivers. Blue light semiconductor lasers use quantum wells.

Because of their quasi-two-dimensional nature, electrons in quantum wells have a density of states as a function of energy that has distinct steps, versus a smooth square root dependence that is found in bulk materials. Additionally, the effective mass of holes in the valence band is changed to more closely match that of electrons in the valence band. These two factors, together with the reduced amount of active material in quantum wells, leads to better performance in optical devices such as laser diodes. As a result, quantum wells are used widely in diode lasers, including red lasers for DVDs and laser pointers, infra-red lasers in fiber optic transmitters, or in blue lasers. They are also used to make HEMTs (high electron mobility transistors), which are used in low-noise electronics. Quantum well infrared photodetectors are also based on quantum wells and are used for infrared imaging.

By doping either the well itself or preferably, the barrier of a quantum well with donor impurities, a two-dimensional electron gas (2DEG) may be formed. Such a structure creates the conducting channel of a HEMT and has interesting properties at low temperature. One such feature is the quantum Hall effect, seen at high magnetic fields. Acceptor dopants can also lead to a two-dimensional hole gas (2DHG).

Saturable absorber

A quantum well can be fabricated as a saturable absorber using its saturable absorption property. Saturable absorbers are widely used in passively mode locking lasers. Semiconductor saturable absorbers (SESAMs) were used for laser mode locking as early as 1974 when p-type germanium was used to mode lock a CO2 laser which generated pulses 500 ps.

Modern SESAMs are III-V semiconductor single quantum well (SQW) or multiple quantum wells (MQW) grown on semiconductor distributed Bragg reflectors (DBRs). They were initially used in a resonant pulse modelocking (RPM) scheme as starting mechanisms for Ti:sapphire lasers which employed KLM as a fast saturable absorber. RPM is another coupled-cavity mode-locking technique. Different from APM lasers that employ non-resonant Kerr-type phase nonlinearity for pulse shortening, RPM employs the amplitude nonlinearity provided by the resonant band filling effects of semiconductors.

SESAMs were soon developed into intracavity saturable absorber devices because of more inherent simplicity with this structure. Since then, the use of SESAMs has enabled the pulse durations, average powers, pulse energies and repetition rates of ultrafast solid-state lasers to be improved by several orders of magnitude. Average power of 60 W and repetition rate up to 160 GHz were obtained. By using SESAM-assisted KLM, sub-6 fs pulses directly from a Ti:sapphire oscillator was achieved.

A major advantage SESAMs have over other saturable absorber techniques is that absorber parameters can be easily controlled over a wide range of values. For example, saturation flu-

ence can be controlled by varying the reflectivity of the top reflector while modulation depth and recovery time can be tailored by changing the low-temperature growing conditions for the absorber layers. This freedom of design has further extended the application of SESAMs into mode-locking of fibre lasers where a relatively high modulation depth is needed to ensure self-starting and operation stability. Fibre lasers working at $\approx 1\ \mu m$ and $1.5\ \mu m$ were successfully demonstrated.

Thermoelectrics

Quantum wells have shown promise for energy harvesting as thermoelectric devices. They are claimed to be easier to fabricate and offer the potential to operate at room temperature. The wells connect a central cavity to two electronic reservoirs. The central cavity is kept at a hotter temperature than the reservoirs. The wells act as filters that allow electrons of certain energies to pass through. In general, greater temperature differences between the cavity and the reservoirs increases electron flow and output power. An experimental device delivered output power of about $0.18\ W/cm^2$ for a temperature difference of 1 K, nearly double the power of a quantum dot energy harvester. The extra degrees of freedom allowed larger currents. Its efficiency is slightly lower than the quantum dot energy harvesters. Quantum wells transmit electrons of any energy above a certain level, while quantum dots pass only electrons of a specific energy.

One possible application is to convert waste heat from electric circuits, e.g., in computer chips, back into electricity, reducing the need for cooling and energy to power the chip.

Solar Cell

Quantum wells have been proposed to increase the efficiency of solar cells. The theoretical maximum efficiency of traditional single-junction cells is about 34%, due in large part to their inability to capture many different wavelengths of light. Multi-junction solar cells, which consist of multiple p-n junctions of different bandgaps connected in series, increase the theoretical efficiency by broadening the range of absorbed wavelengths, but their complexity and manufacturing cost limit their use to niche applications. On the other hand, cells consisting of a p-i-n junction in which the intrinsic region contains one or more quantum wells, lead to an increased photocurrent over dark current, resulting in a net efficiency increase over conventional p-n cells. Photons of energy within the well depth are absorbed in the wells and generate electron-hole pairs. In room temperature conditions, these photo-generated carriers have sufficient thermal energy to escape the well faster than the recombination rate. Elaborate multi-junction quantum well solar cells can be fabricated using layer by layer deposition techniques such as molecular beam epitaxy or chemical vapour deposition. It has also been shown that metal or dielectric nanoparticles added above the cell lead to further increases in photo-absorption by scattering incident light into lateral propagation paths confined within the multiple quantum well intrinsic layer.

Remarks

This program calculates various different important result based on user input data. The way that the program is designed, it can calculate all of the parameters with fair accuracy of any hypothetical double heterostructure based on user input. However there are some limitations to this program in analysis of quantum wells. They have been omitted for a fairly accurate user friendly interface.

1. Effect of excitons has been neglected.In scheme of things, Exciton effects can indeed be ignored and yet still fairly accurate results can be obtained for emission spectrum.

2. Although it is hypothetically possible to calculate results of program fairly accurately using data of any double heterostructure, it should be noted that not all double heterostructures are quantum wells. So the program cannot differenciate between direct and indirect bandgap semiconductors.

   For example, Al(x)Ga(1-x)As is a direct bandgap semiconductor for values of x>0.4 and hence it is required for AlGaAS GaAs quantum well that the value of x remains less than 0.4. Though program calculates results for x>0.4 as well based on user input, it should be noted that it has no practical implications

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