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Analysis of a Finite Quantum Well

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***Abstract*— In this paper one dimensional (1D) quantum confinement in a Finite Quantum Well (FQW) is analyzed through a simulator using MATLAB. A particle behavior inside a FQW is discussed and analyzed. The effect of various parameters such as well boundary thickness, depth of the well and width of the well are discussed. The results are compared with the Infinite Quantum Well (IQW). Different types of potential structure's behavior can be analyzed by using this simulator which is very useful before fabrication.**

***Keywords*—Finite quantum well, infinite quantum well, quantum confinement, quantum tunneling.**

I. INTRODUCTION

Now a day, the buzzing word is the quantum confinement. Quantum effect that is designed to trap carriers within a very small space is known as quantum confinement. For certain application or research we need to change the electrical or optical property of a material and the efficient way to do so is the quantum confinement. When the diameter of a particle is the same as the magnitude of the electron wave function only then the quantum effect is observed. When the size of the confining structure is comparable with the wavelength of the particle the electronic and optical properties are changed. Quantum confining can be done in three different ways such as three dimensional (3D) when confined in a quantum dot, two dimensional (2D) when confined in a quantum wire and one dimensional (1D) when confined in the quantum well. 1D quantum well (QW) is well discussed theoretically in [1]. In this paper the particle (electron) behaviour in a finite quantum well is analysed quantitatively through simulations. Here different parameters of a 1D finite quantum well such as the thickness, depth and width are varied and the behaviour is observed. These parameters variations are done quantitatively, which is very useful to consider prior to any fabrication. Finally the results are compared with the infinite quantum well.

II. QUANTUM WELL (QW)

A potential well having only discrete energy values is known as a quantum well (QW). 1D confinement is possible in QW. When the QW thickness is comparable to the carrier wavelength only then the confinement is possible.

A. *Infinite Quantum Well (IQW)*

When the depth of the potential well is infinite it is called infinite quantum well (IQW). An IQW can be defined (Fig.1) mathematically as-

$$U(x) = \begin{cases} \infty, & x \le 0, \\ 0, & 0 < x < L, \\ \infty, & x \ge L. \end{cases} \quad (1)$$

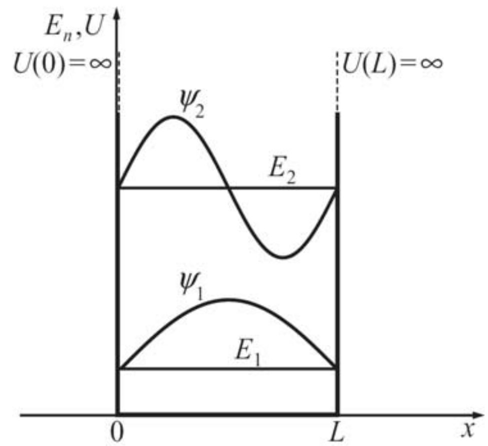

Figure 1. Infinite Quantum Well [1].

An infinite QW is shown in Fig.1 where E_1 and E_2 are the stationary energy states, ψ_1 and ψ_2 are the corresponding wave functions and the QW is infinite in depth. From the definition of a QW we know that the electrons in the potential well or QW have only certain discrete values of allowed energies. These energies can be found through the formula as [1]-

$$E_n = \frac{\hbar^2 k_n^{\ 2}}{2m} = \frac{\pi^2 \hbar^2}{2mL^2} n^2 = \frac{n^2 h^2}{8mL^2} \quad (2)$$

Where E_n is the electron energy, m is the mass of the electron, L is the width of the well, n is the electron energy state. The wave function of the electron in QW is defined as [1]-

$$\psi_n(x) = \sqrt{2/L}\,\sin\left(\frac{n\pi x}{L}\right) \quad (3)$$

B. *Finite Quantum Well (FQW)*

When the depth of the potential well is finite it is called finite quantum well (FQW). An FQW can be defined (Fig.2) mathematically as-

$$U(x) = \begin{cases} U_0, & x \le 0, \\ 0, & 0 < x < L, \\ U_0, & x \ge L. \end{cases} \quad (4)$$

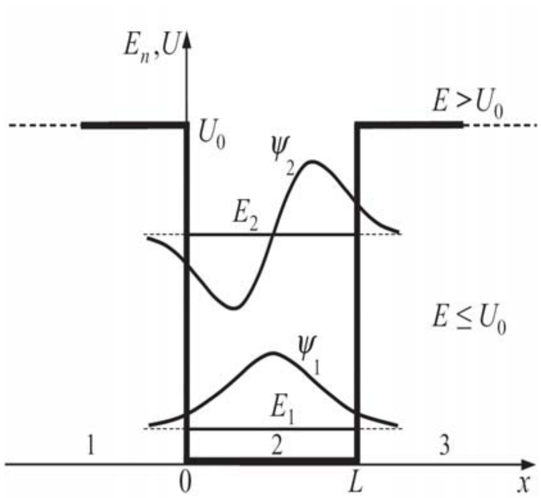

Figure 2. Finite Quantum Well [1].

A finite QW is shown in Fig.2 where E_1 and E_2 are the stationary energy states, ψ_1 and ψ_2 are the corresponding wave functions and the QW is finite in depth. In case of the FQW the discrete energy states can be represented as in [1]-

$$E_n \approx \frac{\pi^2 \hbar^2 n^2}{2m\left(L + \hbar\sqrt{2/(mU_0)}\right)^2} \quad (5)$$

Alternately we can represent the equation as in [2]-

$$2\sqrt{(U_0 - E)E} = (2E - U_0)\tan\left(\sqrt{\frac{2mEL^2}{\hbar^2}}\right) \quad (6)$$

Where-

Outside of the well the wave function is not zero but for infinite case it is zero. So we have-

$$\Delta x^{finite} > L$$

And from the uncertainty principle we have-

$$\Delta p^{finite} x < \Delta p^{\infty} x$$

As described in [2] for FQW the average value of momentum is less than IQW. As a consequence the kinetic energy inside the well is less for FQW than IQW. Moreover, due to the non-zero value of wave function outside of the FQW there exist the possibility to find the particle there and this is the result of tunneling.

III. Simulation & Results

The simulation is done by calculating the stationary states for an electron particle with an effective mass of 10% of the rest mass with certain width and depth by using MATLAB. The algorithm for this simulation is shown in Fig.3.

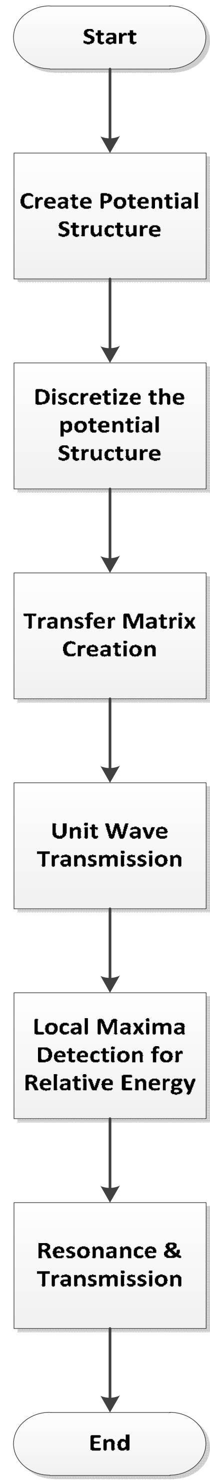

Figure 3. Simulation algorithm flowchart.

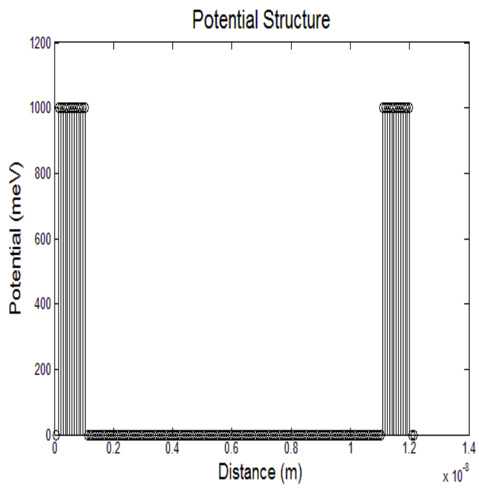

Figure 4. Analyzed Finite Quantum Well.

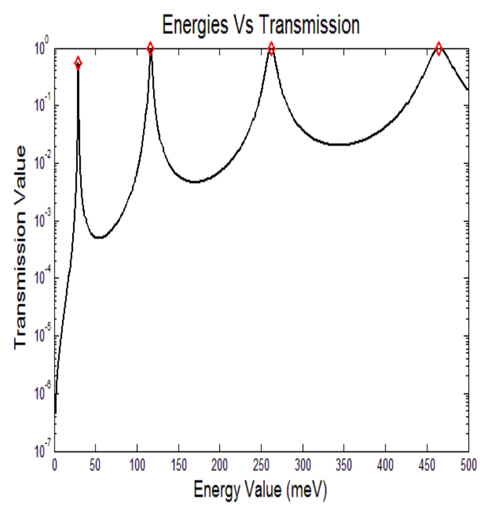

Figure 5. Resonances & transmissions.

For the simulation purpose first of all the potential structure is defined as FQW. Then discretization of the structure is done for calculable transfer matrix as a product of individual propagation matrix as well as the interface matrix. Here it is considered that the particle wave (unit wave function) is coming from right to left. After that the local maxima for relative energy detection was done by bisection method. Finally the resonances and transmissions are detected. The steps of the algorithm are given in Fig.3. The energy values corresponding to the local maximas of the transmission are considered as the stationary states. The structure that was analyzed is given in Fig.4.

In Fig.4 the analyzed finite QW is shown where the finite depth of the well is 1000 meV and the width is in nm size. This FQW structure was varied in depth as well as the boundaries to check the effect on energy states.

In Fig.5 the resonances and corresponding transmissions are shown. In the FQW when there is a resonance inside the QW there will be a corresponding transmission. Here to find the corresponding resonance peak, bisection method was used. As the transfer matrix approach is used for this analysis, so the approximation of an arbitrary potential field is done through step wise approximation. The time independent Schrodinger equation with a constant potential (V_0) is-

$$\hat{H}|\Psi\rangle = E|\Psi\rangle$$

$$\Rightarrow -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V_0\psi = E\Psi \qquad (7)$$

Equation (7) is an ordinary differential equation and the characteristic equation is-

$$-\frac{\hbar^2}{2m}\lambda^2 = \left(E - V_0\right)$$

Where E is the energy, m is the mass of the particle. So there are two conditions to consider for the solution-

$E > V_0$ and $E < V_0$. The general solutions will be-

$$\Psi = A_0 e^{ikx} + B_0 e^{-ikx} \qquad (8)$$

Where, $k = \frac{\sqrt{2m(E - V_0)}}{\hbar}$ and

$$\Psi = A_0 e^{-k'x} + B_0 e^{k'x} \qquad (9)$$

Where, $k' = \frac{\sqrt{2m(V_0 - E)}}{\hbar}$

In (8) the first term of the right hand side is called forward propagating wave and the second term is called the backward propagating wave. Similarly for (9) the right hand side's first term is known as forward decaying field and second term is known as backward decaying field respectively. In this analysis we are considering multilayered structures.

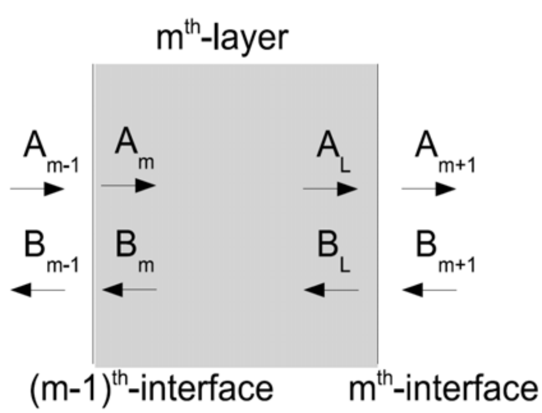

Figure 6. Matrix formation of m^{th} layer structure.

Considering Fig. 6, using the boundary conditions and the continuity at the interface it can written-

$$\begin{bmatrix} A_L \\ B_L \end{bmatrix} = D_m \begin{bmatrix} A_{m+1} \\ B_{m+1} \end{bmatrix} \text{ with } D_m \text{ is the interface matrix.}$$

Now in case of wave propagation in multilayered structure again we consider similar two conditions as it was in constant potential case. Now the potential is multilayered which is denoted as V_m so for first case ($E > V_m$) –

$$A_L = A_m e^{ikd_m} \text{ and } B_L = B_m e^{-ikd_m}$$

Where d_m is the thickness of the layer m. If we write the above equation in matrix form we get-

$$\begin{bmatrix} A_m \\ B_m \end{bmatrix} = P_m^A \begin{bmatrix} A_L \\ B_L \end{bmatrix} \text{ with } P_m^A = \begin{bmatrix} e^{-ikd_m} & 0 \\ 0 & e^{ikd_m} \end{bmatrix}$$

Similarly for the second case ($E < V_m$) –

$$\begin{bmatrix} A_m \\ B_m \end{bmatrix} = P_m^B \begin{bmatrix} A_L \\ B_L \end{bmatrix} \text{with } P_m^B = \begin{bmatrix} e^{k'd_m} & 0 \\ 0 & e^{-k'd_m} \end{bmatrix}$$

Where P is the propagation matrix. So for the complete structure we can write-

$$\begin{bmatrix} A_1 \\ B_1 \end{bmatrix} = T \begin{bmatrix} A_{n+2} \\ B_{n+2} \end{bmatrix} \quad (10)$$

Where transfer matrix-

$$T = P_1 D_1 P_2 D_2 P_3 D_3 .... P_{n+1} D_{n+1} P_{n+2}$$

So the transfer matrix is the combination of propagation matrix and interface matrix. When the energy is determined, using the transfer matrix we obtained the normalized squared modulus of wave functions of different modes which are shown in Fig. 7.

The mode number and their corresponding energies are given in Table I. It is observed that when the mode number is increasing at the same time the energies are also increasing. These energies also depend on the QW structure. The effects of various parameter of the well will be discussed in the following section.

TABLE I. MODES & ENERGIES

Mode Number	Energy (meV)
0	28.9999
1	116.4999
2	261.9374
3	464.8749

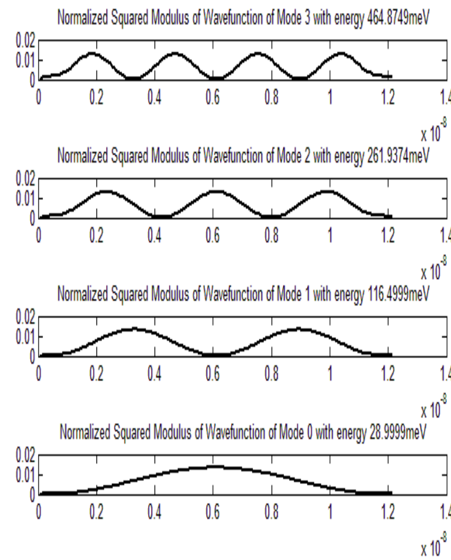

Figure 7. Normalized squared modulus of wave functions of different modes.

A. *Effect of Boundaries Thickness*

For this analysis the values of depth and width of the FQW was fixed i.e. depth & width were constant. The result of this boundaries thickness change is shown in Table II.

TABLE II. THICKNESS VARIATION

Boundaries Thickness (nm):	**0.2**	**0.5**	**1**
Eigen Values (meV)			
E_1	65	83	93
E_2	348	361	371
E_3	903	867	828

From the result it is clear that the change of boundaries thickness affect a lot on energy states. For the initial states the energy is increasing but for higher energy states the energy is decreasing.

B. *Effect of Well's Depth*

For the next analysis the boundaries thickness and width were constant and the depth was varied. The result is given in Table III.

TABLE III. DEPTH VARIATION

Depth (meV):	**100**	**500**	**1000**
Eigen Values (meV)			
E_1	41	75	93
E_2	-	315	371
E_3	-	-	828

When the depth is just 100 meV, only one energy state exists. But with the increment of the depth the number of energy states is also increasing.

C. *Effect of Well's Width*

Finally the boundaries thickness and depth were made constant and the width of the FQW was varied. The result is shown in Table IV.

TABLE IV. WIDTH VARIATION

Width (nm):	**1**	**3**	**5**
Eigen Values (meV)			
E_1	666	198	93
E_2	-	779	371
E_3	-	-	828

From the analysis we can see that the same type of effect is observed for the width variation as it was for depth variation. But the difference is that there is a change in the value of the energy. The result is similar as it is described in [3].

D. *Comparison*

For the comparison purposes we have compared the FQW with IQW as mentioned in Table V. From the comparison we can see that for the IQW each state's energy is higher than the FQW. And the result is similar that was found in [2]. One more comparison is the quantum tunneling effect. The quantum mechanical phenomenon where a carrier or a particle tunnels through a barrier which is not explainable by classical physics is known as the quantum tunneling (as example the working principle of the tunnel diode). For the case of IQW there is no quantum tunneling but for FQW there is quantum tunneling. In Fig. 2 the quantum tunneling is shown for FQW. Moreover the wave functions of the FQW are more spread than the wave functions in IQW [4]. This is another consequence of the quantum tunneling.

TABLE V. COMPARISON: FQW & IQW

Well:	**FQW (Simulated)**	**IQW (Calculated)**
Boundaries Thickness (nm):	1.5	∞
Depth (eV):	10	∞
Width (nm):	5	5
Eigen Values (meV)		
E_1	128.5	150.5
E_2	514	602
E_3	1154.5	1355
E_4	2047	2409
E_5	3187.5	3764.5
E_6	4567	5403
E_7	6169.75	7378
E_8	7961.75	9637

IV. APPLICATIONS

By using this simulator a lot of quantum well based devices can be simulated before the fabrication. Highly flexible implementation of different structures can be realized through this simulator.

V. CONCLUSION

The simulation is done through MATLAB. From the analysis of FQW we have the following observations- increasing the thickness of the boundaries the eigen energies changes, by increasing the depth, the values of bound energies increase and by increasing the width, the eigen energies increase but their values decrease. As the whole analysis is done quantitatively it is very much useful to consider before any fabrication. Because the fabrication process of any device based on QW is so difficult and costly. So it will be a great help for them to have an idea, what happens if the parameters are varied in case of finite quantum well and what are the effects due to this. As a result the fabrication or design of any QW based device can be done precisely.

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REFERENCES

[1] V.V.Mitin, D.I.Sementsov, N.Z.Vagidov, *Quantum Mechanics for Nanostructures*, Cambridge University Press, 2010.

[2] V. Lindberg, "Finite Square Well," Available: http://www.people.rit.edu.

[3] B.R.Nag, *Physics of Quantum Well Devices*, Kluwer Academic Publishers, 2002.

[4] C.L.Tang, *Fundamentals of Quantum Mechanics for Solid State Electronics and Optics*,Cambridge University Press, 2005.