

Time-Independent Schrödinger equation using analytical and numerical methods for
different quantum mechanical potentials



By
Nouman Ahmad Khan
CIIT/FA16-BPH-035/ISB

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different quantum mechanical potentials

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Nouman Ahmad Khan
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to the Department of

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Name	Registration Number
Nouman Ahmad Khan	CIIT/FA16-BPH-035/ISB

Supervisor:

Dr. Javed Akram
Assistant Professor

Department of Physics
CUI, Islamabad Campus

Co-Supervisor:

Dr. Rehmatullah Khattak
Assistant Professor

Department of Physics
CUI, Islamabad Campus



Signature: _____
Nouman Ahmad Khan (CIIT/FA16-BPH-035/ISB)



COMSATS University Islamabad

Final
Approval

This thesis titled

Time-Independent Schrödinger equation using analytical and numerical methods for different quantum mechanical potentials

Submitted for the Degree of BS-Physics

By

Nouman Ahmad Khan

CIIT/FA16-BPH-035/ISB

Has been approved

for

COMSATS University, Islamabad

External Examiner: _____

Supervisor: _____

Dr. Javed Akram
Assistant Professor,
Department of Physics
COMSATS University Islamabad

Co-Supervisor: _____

Dr. Rehmat-ullah Khattak
Assistant Professor,
Department of Physics
COMSATS University Islamabad

HoD: _____

Prof. Dr Muhammad Anis-ur-Rehman
Professor,
Department of Physics
COMSATS University Islamabad

Declaration

I hereby declare that this project neither as a whole nor as a part thereof has been copied out from any source. It is further declared that I have developed this thesis and the accompanied report entirely on the basis of my personal efforts made under the sincere guidance of my supervisor. No portion of the work presented in this report has been submitted in support of any other degree of qualification of this or any other University or Institute of learning, if found I shall stand responsible.



Date: July 28, 2020

Signature of Student:

Nouman Ahmad Khan
CUI/FA16-BPH-035/ISB

Certificate

It is certified that Nouman Ahmad Khan (Registration No. CIIT/FA16-BPH-035/ISB) has carried out all the work related to this thesis under my supervision at the Department of Physics, COMSATS University Islamabad and the work fulfills the requirement for award of BS degree.

Date: July 28, 2020

Supervisor:



Dr. Javed Akram
Assistant Professor
Department of Physics
CUI Islamabad

Co-Supervisor:



Dr. Rehmat-ullah
Assistant Professor
Department of Physics
CUI Islamabad

Head of Department:

Prof. Dr Muhammad Anis-ur-Rehman
Professor
Department of Physics
CUI Islamabad

Every challenging work need effort as well as guidance of elders especially those who are very close to your heart. My humble effort I dedicate to my dear and loving

Father Ashfaq Khan
&
Mother

whose affection, love, encouragement and prayers for days and nights made me able to get such success and honor. I also want to dedicate it to my whole family, without their support none of my success would be possible.

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Abstract

Time-Independent Schrödinger wave Equation is a cornerstone of quantum physics and governs all phenomena of the microscopic world. This thesis highlights the significance of Time-Independent Schrödinger wave equation and also describes how wave-functions and probabilities of a particle changes in different quantum mechanical potentials. The practical significance of these potentials is also discussed in this research. In this thesis, analytical skills and numerical technique like Finite-difference method is used to solve the Time-Independent Schrödinger wave Equation for different quantum mechanical potentials e.g. Square-Well, Harmonic oscillator and Double-Well Potential. Research problem solved by using analytical methods and than numerical simulation techniques are build by using a smart computer programming tool that allows us to work quickly and integrate systems more effectively known as Python programming. Also the Analytical findings are analyzed with the numerical simulations by comparing Eigen-energies, wave-packets and by plotting our results.

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Chapter 1

Introduction

1.1 Quantum Mechanics

With the development of quantum mechanics has pushed many investigations for solving the puzzle of atomic spectra, wave particle duality. Quantum mechanics explained the mathematical equations and explanations for very small particles that the classical mechanics could not explain. In classical mechanics, we say that certain particle or thing is at certain place, however in Quantum mechanics we can't say that particle is on its place but we talk about probability of particle, means that there are certain chances of particles to be there at certain position.

The main aim of this thesis is to compare the analytical and numerical results of different Quantum mechanical potentials.

1.2 Methodology

Methodology is the system of methods used in a particular field. Research methodology specifies the technique used to identify or process the information about a specific topic of research field. In our thesis, Research methodology consists of two techniques, first one is “**Analytical Method**” and second is “**Numerical Method**”. Both are discussed in detail in next sections.

1.3 Analytical Method

First step is to solve the quantum potentials using analytical approach. The exact solution for exact Schrödinger equation play an important role in quantum mechanics. Since the wave function contains all the necessary information to describe a quantum system. However, the Schrödinger equation can be solved for few quantum mechanical potentials.

1.3.1 Schrödinger Equation

On an atomic scale, all particles exhibit a wave-like behavior. Particles can be represented by wavefunctions that obey a differential equation, the Schrödinger Wave Equation which relates spatial coordinates. You can gain valuable insight into quantum mechanics by studying the solutions to the one-dimensional Time-Independent Schrödinger wave equation.

A wave equation that describes the behavior of an electron was developed by Schrödinger in 1925. He introduced a wavefunction $\psi(x)$. This is a purely mathematical function and does not represent any physical entity. An interpretation of the wave function was given by Born in 1926 who suggested that the quantity $|\psi(x)|^2$ represents the probability density of finding an electron. For the one dimensional case, the probability of finding the electron somewhere between x_1 and x_2 is given by

$$prob = \int_{x_1}^{x_2} \psi(x)\psi^*(x)dx \quad (1.1)$$

where, ψ^* is the complex conjugate of the wavefunction ψ . The value of Probability must lie between 0 and 1 and so when we integrate over all space, the probability of finding the particle must be 1.

$$\int_{-\infty}^{+\infty} \psi(x)\psi^*(x)dx = 1 \quad (1.2)$$

In our project, we will solve 1-D Schrödinger equation for three different quantum mechanical potentials.

We can see how the time-independent Schrödinger Equation in one dimension is plausible for a particle of mass m , whose motion is governed by a potential energy function $U(x)$ by starting with the classical one dimensional wave equation and using the de Broglie relationship,

- Classical wave eq:

$$\frac{\partial\psi^2(x,t)}{\partial x^2} - \frac{1}{v^2} \frac{\partial\psi^2(x,t)}{\partial t^2} = 0 \quad (1.3)$$

- Momentum(De-Broglie):

$$p = mv = \frac{h}{\lambda} = hk \quad (1.4)$$

- **Kinetic Energygy:**

$$K = \frac{1}{2}mv^2 \quad (1.5)$$

- **Total Energygy:**

$$E = K(x) - U(x) \quad (1.6)$$

combining all these equations, we get Schrödinger wave equation,

$$\boxed{-\frac{\hbar^2}{2m} \frac{d^2\Psi}{dx^2} + V\Psi = E\Psi} \quad (1.7)$$

We solve the linear Schrödinger equation and get normalized wavefunction and Energy equation 1.7. Our goal is to find solutions of this form of the Schrödinger Equation for a potential energy function which traps the particle within a region. The negative slope of the potential energy function gives the force on the particle. For the particle to be bound the force acting on the particle is attractive. The solutions must also satisfy the boundary conditions for the wavefunction. The probability of finding the particle must be one, therefore, the wavefunction must approach zero as the position from the trapped region increases. The imposition of the boundary conditions on the wavefunction results in a discrete set of values for the total energy E of the particle and a corresponding wavefunction for that energy, just like a vibrating guitar string which has a set of normal modes of vibration in which there is a harmonic sequence for the vibration frequencies.

1.4 Numerical Approach

In this method, we use tool to do our simulations i.e, Python programming language or MATLAB .

1.4.1 Python

It is programming language that let us work more quickly and integrate your systems more effectively.

we use python programming language as a tool to do our work more efficiently and effectively. We used to analyse numerical data using this tool for example plotting our results and comparing numerical and analytical findings.



Figure 1.1: python logo

1.4.2 Finite Difference Method

The finite-difference method is a technique we used in numerical simulations. With help of tailor series, we approximate the second derivative in 1-D Schrödinger wave equation.

$$H\psi = E\psi \quad (1.8)$$

$$-\frac{\hbar^2}{2m} \frac{d^2\Psi}{dx^2} + V\Psi = E\Psi \quad (1.9)$$

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2}f''(x) + \dots \quad (1.10)$$

using this series upto first order term,

$$f(x+h) - f(x) = hf'(x) \quad (1.11)$$

$$f'(x) = \frac{f(x+h) - f(x)}{h} \quad (1.12)$$

or we can also write it as eq 1.17.

Similarly, for second derivative, we approximate our series upto second order term.

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2}f''(x) \quad (1.13)$$

$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2}f''(x) \quad (1.14)$$

adding both eq 1.13 and 1.14,

$$f(x+h) + f(x-h) = 2f(x) + h^2f''(x) \quad (1.15)$$

$$f''(x) = \frac{f(x+h) + f(x-h) - 2f(x)}{h^2} \quad (1.16)$$

which is similar to eq 1.19.

So, from finite difference method the definitions of first and second derivatives of function $y(x)$ are,

$$\frac{dy}{dx}\Big|_{x(n-\frac{1}{2})} \approx \frac{y_n - y_{n-1}}{\Delta x} \quad (1.17)$$

$$\frac{d^2y}{dx^2}\Big|_{x_n} \approx \frac{1}{\Delta x} \left[\frac{dy}{dx}\Big|_{x(n+\frac{1}{2})} - \frac{dy}{dx}\Big|_{x(n-\frac{1}{2})} \right] \quad (1.18)$$

putting values from eq 1.17 we get,

$$\frac{d^2y}{dx^2}\Big|_{x_n} = \frac{y_{n+1} - 2y_n + y_{n-1}}{\Delta x^2}$$

(1.19)

using eq 1.19, we approximate the second derivative of wavefunction in our linear Schrödinger wave equation. After approximation we create matrices upto NxN value and do our numerical simulations using python programming.

After finding wavefunctions, we plot our wavefunctions and also probabilities of particles for a particular potential well.

Chapter 2

Infinite Square Well

Quantum Mechanics is quite different from classical mechanics. In classical mechanics we talk about bigger and real life objects, their position and momentum etc, but in Quantum mechanics we talk about tiny and small particles and their probabilities.

Infinite-Square well is the most simplest case in quantum mechanical systems. This system describes that we have a particle that is trapped inside a box or a well that has zero potential inside it and an infinite potential lies outside the well or the box. This means that the particle cannot escape the well and is confined inside it [4].

This system can also be used to differentiate between classical and quantum mechanical system.

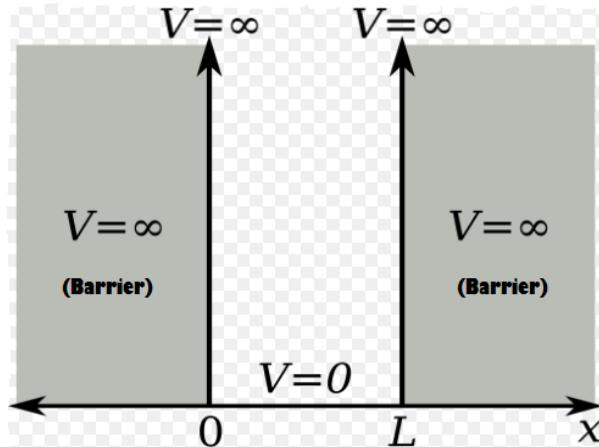


Figure 2.1: infinite square well

In above fig 2.1, infinite square well is shown, having infinite potential on left and right region and zero potential in region) to L. Particle will be trapped in the region of lower potential and can not cross the barrier in any condition due to very very high potential on other sides.

This means that the probability of finding particle will always in the region of zero potential.

2.1 Analytical Method

To solve infinite-square well by this method, we start the mathematical calculation by writing Schrödinger wave equation,

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} - V\psi = E\psi \quad (2.1)$$

in above eq 2.1 we see this this as the potential inside the well is zero, so putting $V=0$ we get,

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} = E\psi \quad (2.2)$$

Now, we use separation of variables technique to solve eq 2.2,

$$\left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \right] \psi = E\psi \quad (2.3)$$

$$\frac{d^2\psi}{dx^2} = -\frac{2m}{\hbar^2} E\psi \quad (2.4)$$

we let,

$$K = \frac{\sqrt{2mE}}{\hbar} \quad (2.5)$$

so eq 2.4 becomes,

$$\frac{d^2\psi}{dx^2} = -K^2\psi \quad (2.6)$$

eq 2.6 is an auxilary equation, we solve it to get roots, we get imaginary roots so our solution will be written as

$$\psi(x) = A \sin(Kx) + B \cos(Kx) \quad (2.7)$$

in order to find values of constants A and B, we apply boundry conditions on equation 2.7

Boundary condition 1:

$$\psi(0) = 0$$

$$\psi(0) = A \sin(0) + B \cos(0) \quad (2.8)$$

we get $B=0$, so eq 2.7 becomes

$$\psi(x) = A \sin(Kx) \quad (2.9)$$

Boundary condition 2:

$$\psi(a)=0$$

$$\psi(a) = A \sin(Ka) \quad (2.10)$$

as $A \neq 0$, so

$$\sin(Ka) = 0 \quad (2.11)$$

$$ka = n\pi \quad (2.12)$$

$$K = \frac{n\pi}{a} \quad (2.13)$$

eq 2.9 becomes,

$$\psi(x) = A \sin\left(\frac{n\pi x}{a}\right)$$

(2.14)

this is our required wavefunction.

Normalizing the wavefunction:

Now, we want normalized value of our wavefunction, so we will normalize it on region of our well width i.e, $0 \rightarrow a$,

$$\int_0^a |\psi|^2 dx = 1 \quad (2.15)$$

$$\int_0^a |A|^2 \sin^2\left(\frac{n\pi x}{a}\right) dx = 1 \quad (2.16)$$

using identity,

$$\sin^2(x) = \frac{1 - \cos(2x)}{2} = 1 \quad (2.17)$$

$$|A|^2 \int_0^a \frac{1 - \cos\left(\frac{2n\pi x}{a}\right)}{2} dx = 1 \quad (2.18)$$

$$|A|^2 \frac{1}{2} \left[\int_0^a dx - \int_0^a \cos\left(\frac{2n\pi x}{a}\right) dx = 1 \right] , \quad (2.19)$$

$$|A|^2 \left[x \Big|_0^a - \left(\frac{a}{2n\pi} \right) \sin\left(\frac{2n\pi x}{a}\right) \Big|_0^a \right] = 2 , \quad (2.20)$$

$$|A|^2 \left[(a - 0) - \left(\frac{a}{2n\pi} \right) (\sin(2n\pi) - \sin(0)) \right] = 2 , \quad (2.21)$$

$$|A|^2 a = 2 , \quad (2.22)$$

$$|A|^2 = \frac{2}{a} , \quad (2.23)$$

$$A = \sqrt{\frac{2}{a}} , \quad (2.24)$$

by putting value of A in eq 2.14 we get normalized wave function, so eq 2.14 becomes,

$$\boxed{\psi(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right)} \quad (2.25)$$

from equation 2.5, we get value of **Energy**,

$$\boxed{E_n = \frac{n^2 \pi^2 \hbar^2}{2ma^2}} \quad (2.26)$$

Above is eigen energy equation of particle trapped in infinite-square well.
For required nth value, we find the eigen energy and wave-function for particle in infinite-square well. We plot the wave-functions using python.

2.2 Numerical Method

In this method, we use python to do mathematical part and than plotting the results. For this analysis, we use **finite difference method** to approximate the second derivative in our Schrödinger wave equation. Finite difference method is done by using matrices, so this is also known as **matrix method**.

in matrix method we represent the operator $\frac{-\hbar^2}{2m} \frac{d^2}{dx^2}$ in form of matrices of N-2 x N-2,
Now, from the equation of finite difference method (discussed earlier in chapter 1)

$$\frac{d^2y}{dx^2}\Big|_{x_n} = \frac{y_{n+1} - 2y_n + y_{n-1}}{\Delta x^2} \quad (2.27)$$

we make matrix.

suppose N=6, than the Matrix of second derivative will be written in the form of 4x4 matrix.

$$[SD] = \frac{1}{\Delta x^2} \begin{bmatrix} -2 & 1 & 0 & 0 \\ 1 & -2 & 1 & 0 \\ 0 & 1 & -2 & 1 \\ 0 & 0 & 1 & -2 \end{bmatrix} \quad (2.28)$$

Question is, why we can't do it using N x N matrices?

The SD matrix size is (N-2) X (N-2) and not NXN because the second derivative of the function can't be evaluated at the end points, n = 1 and n = N, because we apply the boundary conditions at boundaries to add two more digits i.e, 0 at the end. The Kinetic energy matrix [K] is defined as,

$$[K] = C_{se} [SD] \quad (2.29)$$

i.e $C_{se} = \frac{-\hbar^2}{2m}$, for simplicity, we took $\hbar = 1$ and $m=1$, so $C_{se} = \frac{1}{2}$. Now, we can find Hamiltonian matrix,

$$[H] = [K] + [V] \quad (2.30)$$

as the potential is zero inside the well so, the Hamiltonian matrix will be equal to Kinetic energy matrix, i.e, $[H] = [K]$

From

$$[H] |\psi_n\rangle = E_n |\psi_n\rangle \quad (2.31)$$

this is an eigen value equation in matrix form where the action of Hamiltonian matrix results in each value to be the vector $|\psi_n\rangle$ being multiplied by set of number E_n .

These set of E_n is called **Eigen energies** and set of $|\psi_n\rangle$ is called **Eigen Vectors**.

Using these Eigen energies and Eigen vectors, we plot wavefunctions and their probabilities. The wave functions and the probabilities of particle in first three energy levels are shown below,

2.3 Conclusion

Wavefunctions

By comparing numerical and analytical results we conclude that we get exact same numerical and analytical plots for wave functions and probabilities.

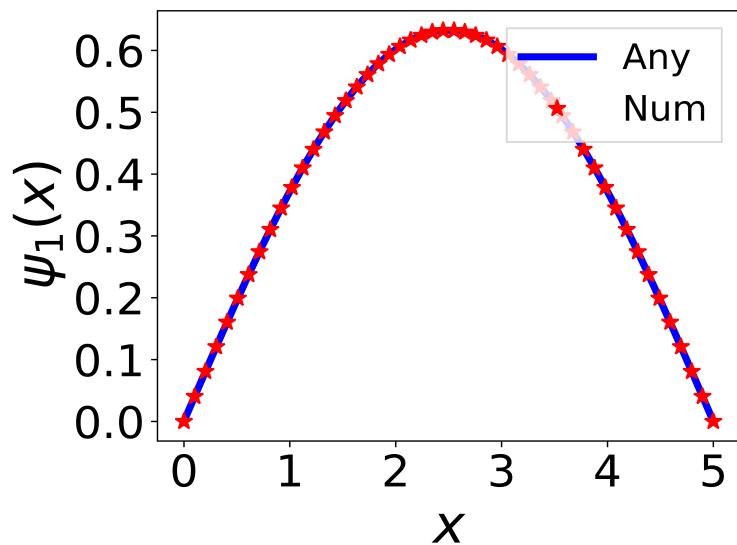


Figure 2.2: Numerical and Analytical wavefunctions plot comparison of Infinite square well for $n=1$

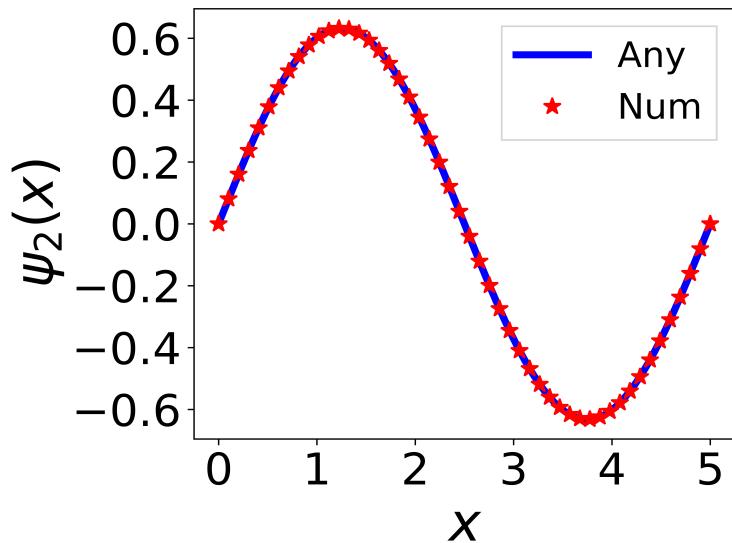


Figure 2.3: Numerical and Analytical wavefunctions plot comparison of Infinite square well for $n=2$

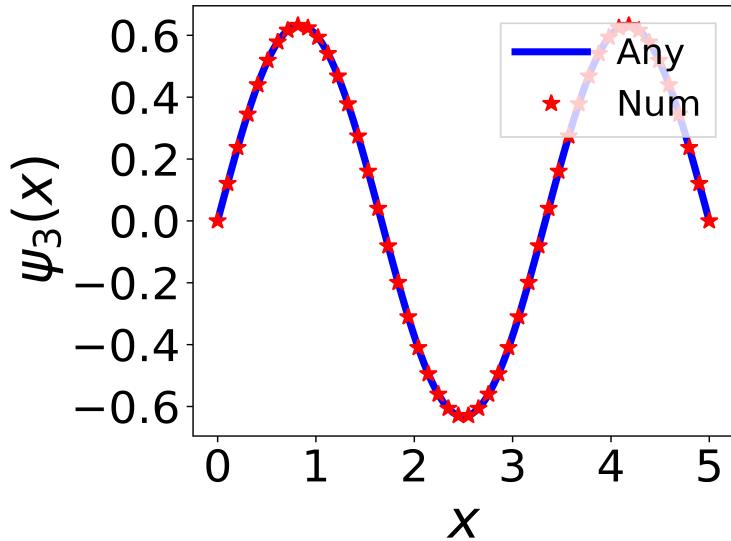


Figure 2.4: Numerical and Analytical wavefunctions plot comparison of Infinite square well for $n=3$

Fig 2.2 shows the wavefunction for ground state of infinite-square well, similarly fig 2.3 and 2.4 shows wavefunction for $n=2$ and $n=3$ respectively. After plotting probabilities of these wavefunctions, we compared their analytical and numerical plots and those matches quite well.

Probabilities

We plot probabilities of particle in infinite-square well. We compare analytical and numerical plots for first three energy states i.e, $n=1, 2$ and 3 .

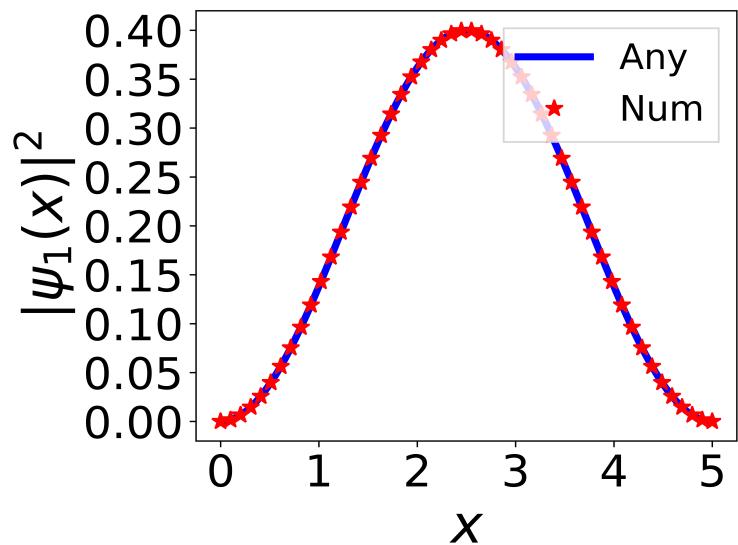


Figure 2.5: Numerical and Analytical Probabilities plot comparison of Infinite square well for $n=1$

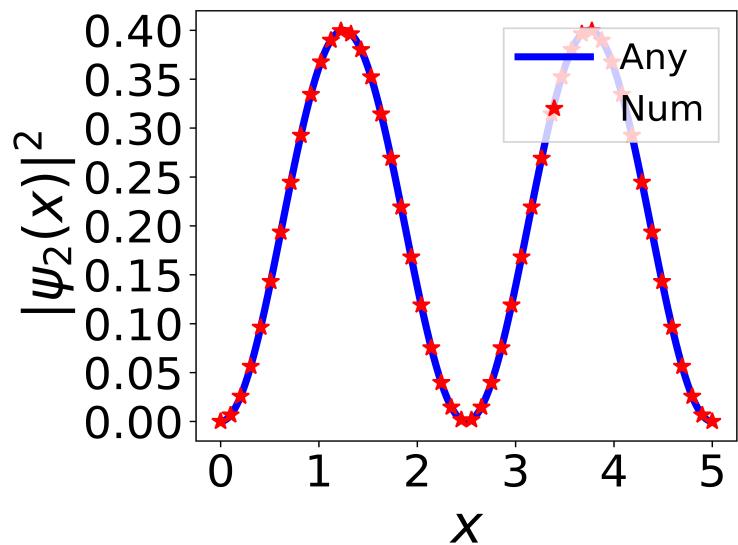


Figure 2.6: Numerical and Analytical Probabilities plot comparison of Infinite square well for $n=2$

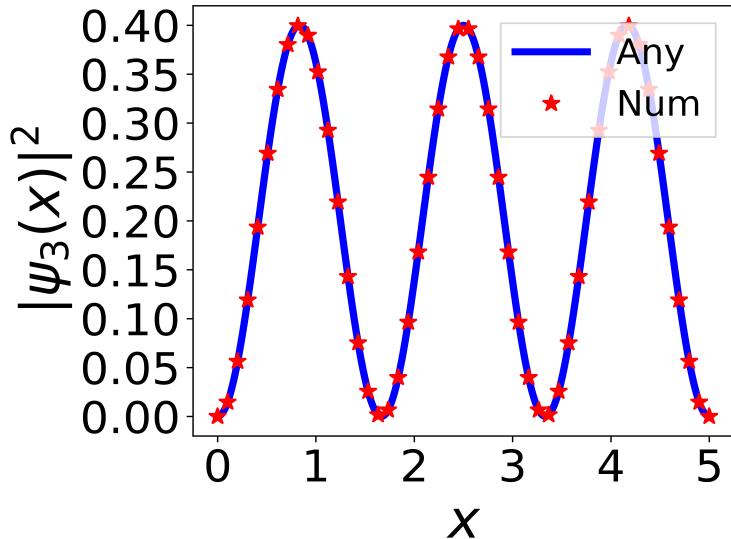


Figure 2.7: Numerical and Analytical Probabilities plot comparison of Infinite square well for $n=3$

In fig 2.5 probability of particle is maximum at center of well, but zero at boundaries because wavefunction is zero at boundaries. In fig 2.6 there are two points having maximum probability and three points having zero probability.

Similarly in fig 2.7, we have three points having maximumm probability. As we go up in energy states, the wavefunction oscillations increases and so probability plot having more points of maximum probabilities.

2.4 Physical Significance of Infinite-Square well

With the development of quantum mechanics, has pushed many investigations for solving the puzzle of atomic spectra, wave-particle duality [1]. The quantum effects can be visualized effortlessly in semiconductor gadgets. This can later result in the layout of new kinds of nanomaterials are defined through quantum phenomena consisting of confinement, superposition and entanglement and so on.

It might be very difficult these days to imagine solid state physics without semiconductor hetero systems. quantum wells, quantum wires and quantum dots and additionally including double hetero-structures they are pretty much exciting topics of studies these days. Quantum wells (QW), wires and dots (QD) has proven very thrilling quantum mechanical effects.

Quantum dots and Quantum wires can be modeled as Infinite square well.

2.4.1 Graphene Quantum Dots (GQD's)

Quantum dots are collections of artificial atoms whose electronic degrees of freedom are quantized, similar to those of an atom, due to the confinement of electrons and holes inside

a quantum well [2].

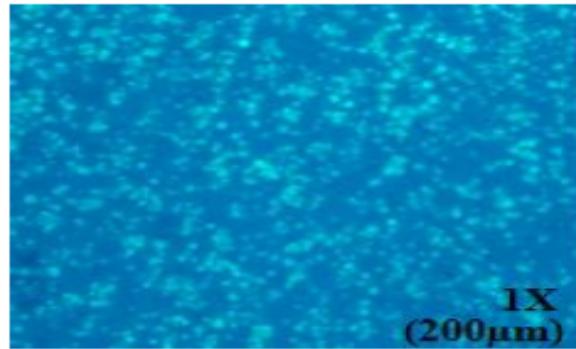


Figure 2.8: The optical image of GQDs

In a semiconductor, these artificial atoms are small boxes of size ranging from 1 nm to 100 nm, capable of holding number of electrons that can be varied as required by varying the number of electrons in the artificial atoms of a semiconductor, many atomic physics experiments have been carried out in this regime which is not feasible to perform in real atoms in real-time scenario. QDs have highly tunable optical and electronic properties, which differ significantly from those of large particles due to which QDs have potential applications in field of electronics, engineering and aerospace industries.

Dimension is defined as minimum number of coordinates used to specify the point within it. Quantum Dot have promising zero dimensions because of their nanoscale size they can be engineered to fabricate particular applications such as nonlinear optical devices (NLO). This scenario is defined as the particle is trapped and can not escape out of very high potential region and this is infinite-square well.

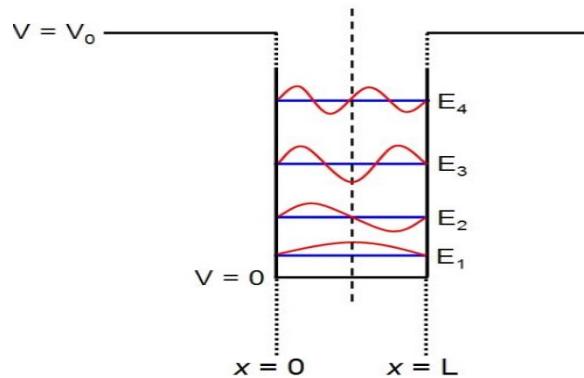


Figure 2.9: Infinite-Square well

Chapter 3

Harmonic Oscillator

Harmonic motion is one of the most important types of motion in physics. The vibration of any type with restoring force equals to Hook's law caused by simple harmonic oscillator with potential having small oscillations at minimum. Almost all potentials in nature have small oscillations at the minimum, including many systems studied in quantum mechanics. Here, harmonic motion plays a fundamental role as a stepping stone in more rigorous applications.

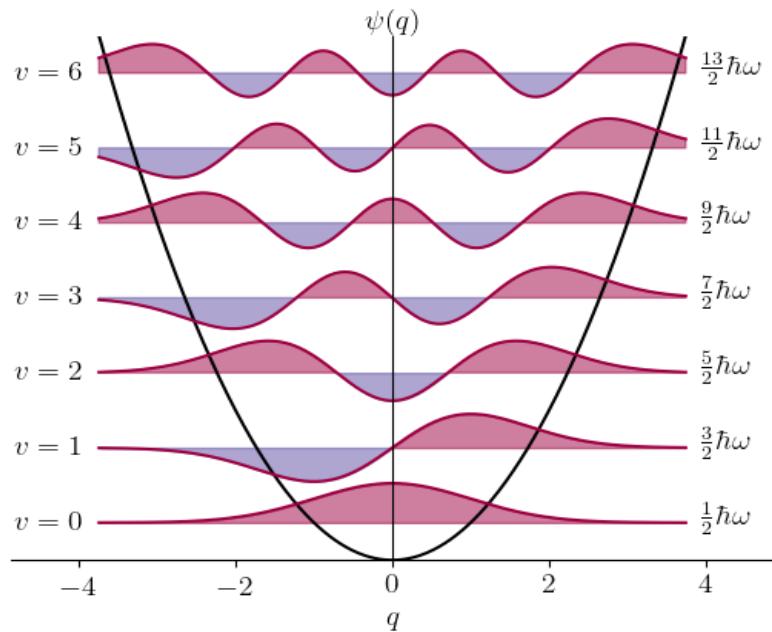


Figure 3.1: 1-D Harmonic Oscillator

3.1 Analytical Method

Again we start from **Schrödinger equation**

$$\boxed{-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + V\psi = E\psi}, \quad (3.1)$$

And the quantum harmonic potential is shown in fig 3.1

$$V(x) = \frac{1}{2}Kx^2 \quad (3.2)$$

$$\omega = \sqrt{\frac{k}{m}} \quad (3.3)$$

Where ω is natural frequency, m is masss of body and k is spring constant

$$V(x) = \frac{1}{2}m\omega^2x^2 \quad (3.4)$$

Now, the Schrödinger equation becomes

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + \frac{1}{2}m\omega^2x^2\psi = E\psi \quad , \quad (3.5)$$

$$\frac{d^2\psi}{dx^2} \left(\frac{2mE}{\hbar^2} - \frac{m^2\omega^2}{\hbar^2}x^2 \right) \psi = 0 \quad (3.6)$$

We can solve this second order differential equation by **power series** method: first step is change of variables so, let

$$y = \sqrt{\frac{m\omega}{\hbar}}x \quad (3.7)$$

Substituting this in eq 3.6 , we get;

$$\frac{d^2\psi(y)}{y^2} + \left(\frac{2E}{\hbar\omega} - y^2 \right) \psi(y) = 0 \quad (3.8)$$

In this Differential equation for small Energy(E) the y^2 term dominates in this case D.E will be

$$\psi''(y) = y^2\psi(y) \quad , \quad (3.9)$$

$$\psi(y) = U(y)e^{\frac{y^2}{2}} \quad (3.10)$$

Now, calculating derivatives of $\psi(y)$ to substitute it in the Schrödinger equation:

$$\psi(y) = U(y)e^{\frac{y^2}{2}} \quad (3.11)$$

$$\frac{d\psi(y)}{dy} = \frac{dU(y)}{dy}e^{\frac{-y^2}{2}} + U(y)(-y)e^{\frac{y^2}{2}} \quad (3.12)$$

$$\frac{d^2\psi(y)}{dy^2} = \frac{d^2U(y)}{dy^2}e^{\frac{-y^2}{2}} + \frac{d\psi(y)}{dy}(-y)e^{\frac{-y^2}{2}} + (-y)\frac{dU(y)}{dy}e^{\frac{-y^2}{2}} + U(y)(-1+y^2)e^{\frac{y^2}{2}} \quad (3.13)$$

Putting $\psi(y)$ and second derivative in eq 3.8, we get

$$\frac{d^2U(y)}{dy^2}e^{\frac{-y^2}{2}} + (-2y)\frac{dU(y)}{dy}e^{\frac{-y^2}{2}} + U(y)(-1+y^2)e^{\frac{-y^2}{2}} + \left(\frac{2E}{\hbar\omega} - y^2\right)U(y)e^{\frac{-y^2}{2}} = 0 \quad (3.14)$$

$$\frac{d^2U(y)}{dy^2}e^{\frac{-y^2}{2}} - 2y\frac{dU(y)}{dy}e^{\frac{-y^2}{2}} - U(y)e^{\frac{-y^2}{2}} + \frac{2E}{\hbar\omega}U(y)e^{\frac{-y^2}{2}} = 0 \quad (3.15)$$

$$\frac{d^2U(y)}{dy^2} - 2y\frac{dU(y)}{dy} - U(y)e^{\frac{-y^2}{2}} + \frac{2E}{\hbar\omega}U(y) = 0 \quad (3.16)$$

$$\frac{d^2U(y)}{dy^2} - 2y\frac{dU(y)}{dy} + \left(\frac{2E}{\hbar\omega} - 1\right)U(y) = 0 \quad (3.17)$$

Now, we have to solve second order D.E for $U(y)$ in order to obtain solution for $\psi(y)$. We begin by using a power series of y as general solution to eq,

$$U(y) = \sum_{n=0}^{\infty} a_n y^n \quad (3.18)$$

$$\frac{dU(y)}{dy} = \sum_{n=1}^{\infty} n a_n y^{n-1} \quad (3.19)$$

$$\frac{d^2U(y)}{dy^2} = \sum_{n=2}^{\infty} (n-1) n a_n y^{n-2} \quad (3.20)$$

Putting derivatives in eq 3.17

$$\sum_{n=0}^{\infty} n a_n y^{n-2} - \sum_{n=1}^{\infty} (2y)(n) a_n y^{n-1} + \left(\frac{2E}{\hbar\omega} - 1\right) \sum_{n=0}^{\infty} a_n y^n = 0 \quad (3.21)$$

$$\sum_{n=0}^{\infty} n a_n y^{n-2} + \left(\frac{2E}{\hbar\omega} - 1 - 2n\right) \sum_{n=0}^{\infty} a_n y^n = 0 \quad (3.22)$$

Now, for simplifying summition, we replace n with $n+2$,

$$\sum_{n=0}^{\infty} (n+2-1)(n+2) a_{n+2} y^{n+2-2} + \left(\frac{2E}{\hbar\omega} - 1 - 2(n+2)\right) \sum_{n=0}^{\infty} a_{n+2} y^{n+2} = 0 \quad (3.23)$$

$$\sum_{n=0}^{\infty} \left[(n+1)(n+2) a_{n+2} + \left(\frac{2E}{\hbar\omega} - 1 - 2n\right) a_n \right] y^{2n} = 0 \quad (3.24)$$

we solve it for a_{n+2} ,

$$a_{n+2} = \frac{2n + 1 - \frac{2E}{\hbar\omega}}{(n+2)(n+1)} a_n \quad (3.25)$$

It gives recurrence relation in terms of a_o . As the value of y is large, n will also be large, the ratio of a_{n+1} and a_n is very close to $2/n$ but limit $2/n$ grows faster than the exponential term $\psi(y)$. So, the series must terminate for our solution. Series terminates if R.H.S=0.
So, it means numerator=0

$$2n + 1 - \frac{2E}{\hbar\omega} = 0 \quad (3.26)$$

$$E = \frac{\hbar\omega}{2}(2n + 1) \quad (3.27)$$

$$\boxed{E = \left(n + \frac{1}{2}\right) \hbar\omega} \quad (3.28)$$

This is energy equation of harmonic oscillator for level n .

Power series solution is incomplete, as individual eigen states of Hamiltonian are not yet made orthogonal. When we do this, we get solution that involves "**Harmite polynomials**".
So, general equation of wavefunction for harmonic Oscillator is

$$\boxed{\psi_n(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n(x) e^{-\frac{m\omega}{2\hbar}x^2}} \quad (3.29)$$

Where, $H_n(x)$ is Harmite polynomials

$$H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n} e^{-x^2} \quad (3.30)$$

and we get, $H_0 = 1$, $H_1 = 2x$, $H_2 = 4x^2 - 2$ in our case $m=1$, $\omega=1$, $\hbar=1$

For ground state $\boxed{n = 0}$,

$$\boxed{\psi_0 = \left(\frac{1}{\pi}\right)^{1/4} e^{\frac{-x^2}{2}}} \quad (3.31)$$

Similarly, for $\boxed{n = 1}$

$$\psi_1 = \left(\frac{1}{\pi}\right)^{1/4} \frac{1}{\sqrt{2}} 2x e^{\frac{-x^2}{2}} \quad (3.32)$$

$$\boxed{\psi_1 = \left(\frac{1}{\pi}\right)^{1/4} \sqrt{2} x e^{\frac{-x^2}{2}}} \quad (3.33)$$

And for $\boxed{n = 2}$

$$\boxed{\psi_2 = \left(\frac{1}{\pi}\right)^{1/4} \frac{1}{\sqrt{8}} (4x^2 - 2) e^{\frac{-x^2}{2}}} \quad (3.34)$$

So, these are the first three wavefunctions of 1-D Harmonic Oscillator. We found these analytically, now in next part we solve them numerically.

3.2 Numerical Method

Again using **Finite-difference method** to approximate the second derivative in our Schrödinger wave equation. Finite difference method is done by using matrices, so this is also known as **matrix method**.

In matrix method we represent the operator $\frac{-\hbar^2}{2m} \frac{d^2}{dx^2}$ in form of matrices of N-2 x N-2, Now, from the equation of Finite-difference method (discussed earlier in chapter 1)

$$\left. \frac{d^2y}{dx^2} \right|_{xn} = \frac{y_{n+1} - 2y_n + y_{n-1}}{\Delta x^2} \quad (3.35)$$

Suppose N=6, than the matrix of second derivative will be written in the form of 4x4 matrix.

$$[SD] = \frac{1}{\Delta x^2} \begin{bmatrix} -2 & 1 & 0 & 0 \\ 1 & -2 & 1 & 0 \\ 0 & 1 & -2 & 1 \\ 0 & 0 & 1 & -2 \end{bmatrix} \quad (3.36)$$

Question is, why we can't do it using N x N matrices?

The SD matrix size is (N-2) X (N-2) and not N X N because the second derivative of the function can't be evaluated at the end points, n = 1 and n = N, because we apply the boundary conditions at boundaries to add two more digits i.e, 0 at the end.

The Kinetic energy matrix [K] is defined as,

$$[K] = C_{se} [SD] \quad (3.37)$$

i.e $C_{se} = \frac{-\hbar^2}{2m}$, for simplicity, we took $\hbar = 1$ and $m=1$, so $C_{se} = \frac{1}{2}$.
Now, we can find Hamiltonian matrix,

$$[H] = [K] + [U] \quad (3.38)$$

We know that the potential of harmonic oscillator is,

$$V(x) = \frac{1}{2}m\omega^2x^2 \quad (3.39)$$

Where for simplicity we took $m = 1$ and $\omega = 1$ so

$$V(x) = \frac{1}{2}x^2 \quad (3.40)$$

Now, we make matrix of potential energy term,
let we take N=6 than matrix will be,

$$[V] = \begin{bmatrix} x^2/2 & 0 & 0 & 0 \\ 0 & x^2/2 & 0 & 0 \\ 0 & 0 & x^2/2 & 0 \\ 0 & 0 & 0 & x^2/2 \end{bmatrix} \quad (3.41)$$

So the Hamiltonian matrix will be equal to sum of Kinetic energy matrix and Potential energy matrix, i.e, $[H] = [K + U]$

From

$$[H] |\psi_n\rangle = E_n |\psi_n\rangle \quad (3.42)$$

This is an eigen value equation in matrix form. Where, the action of Hamiltonian matrix results in each value to be the vector $|\psi_n\rangle$ being multiplied by set of number E_n .

These set of E_n is called **Eigen energies** and set of $|\psi_n\rangle$ is called **Eigen Vectors**.

3.3 Conclusion

Wavefunctions

We plot first three wavefunctions and compared both methods. We found that our wavefunctions for both methods matches quite well.

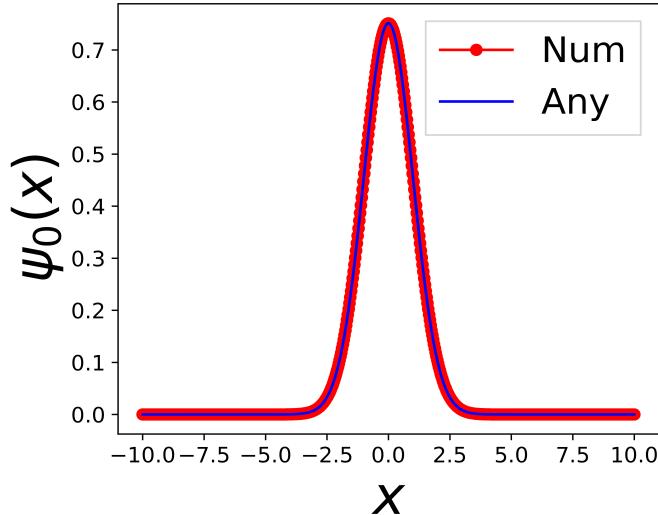


Figure 3.2: Numerical and Analytical plots of wavefunction of Harmonic Oscillator for $n=0$

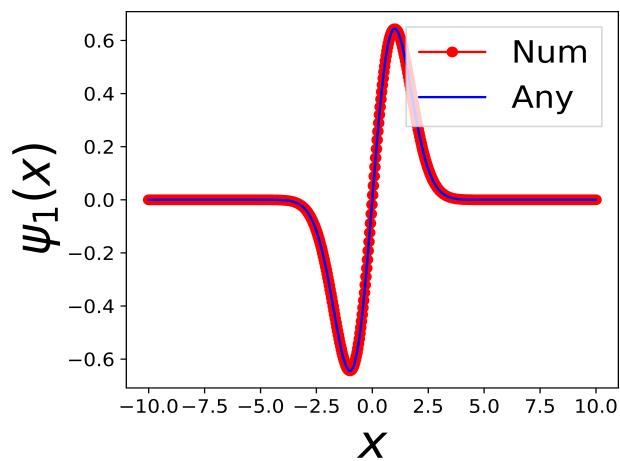


Figure 3.3: Numerical and Analytical plots of wavefunction of Harmonic Oscillator for $n=1$

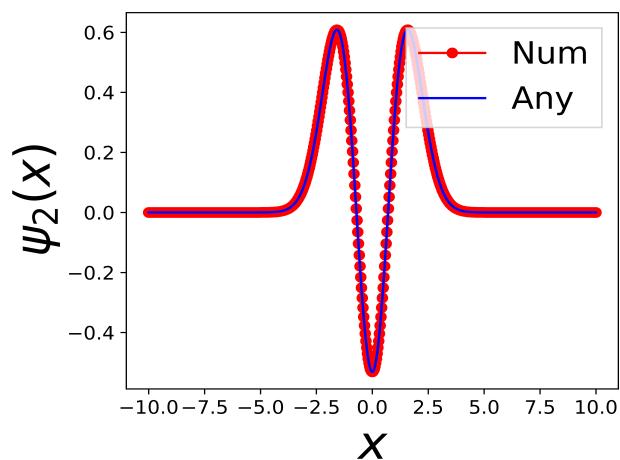


Figure 3.4: Numerical and Analytical plots of wavefunction of Harmonic Oscillator for $n=2$

Blue line shows analytical and Red line shows numerical data. In fig 3.2 we have guassian function for ground state. fig 3.3 shows plot for n=1 having two opposite peaks. similarly in fig 3.4 we have three vertical peaks. We plot probabilites after plotting these wavefunctions.

Probabilities

We also plot probabilities of the paritcle in first three energy states and our results for both methods matches again. We plot probabailities of first three energy states. Blue plot shows analytically plot data and red one shoes numerical method plot.

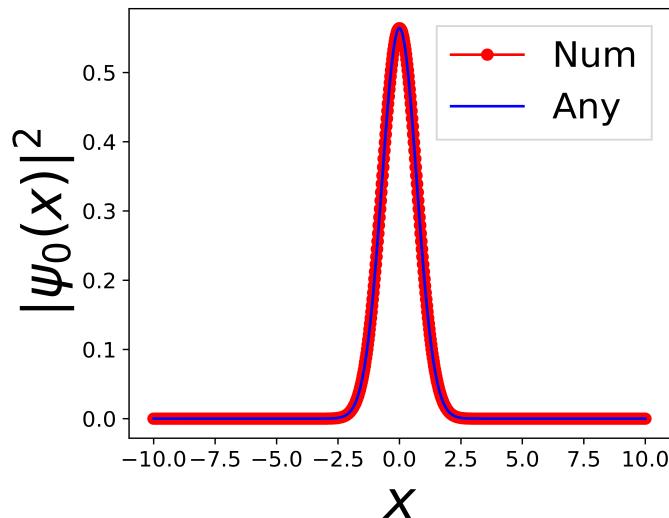


Figure 3.5: Numerical and Analytical plots of probabiility of Harmonic Oscillator for n=0

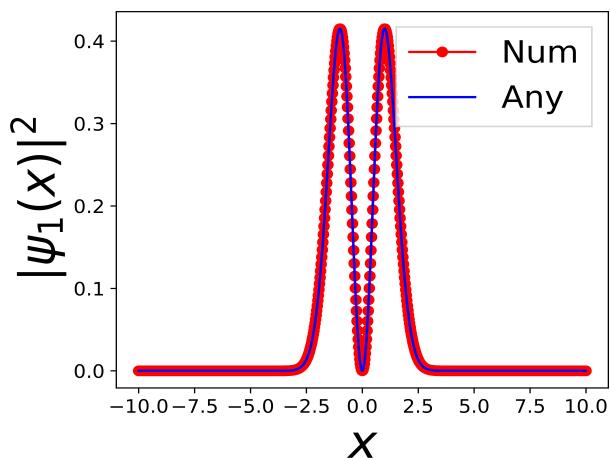


Figure 3.6: Numerical and Analytical plots of probability of Harmonic Oscillator for $n=1$

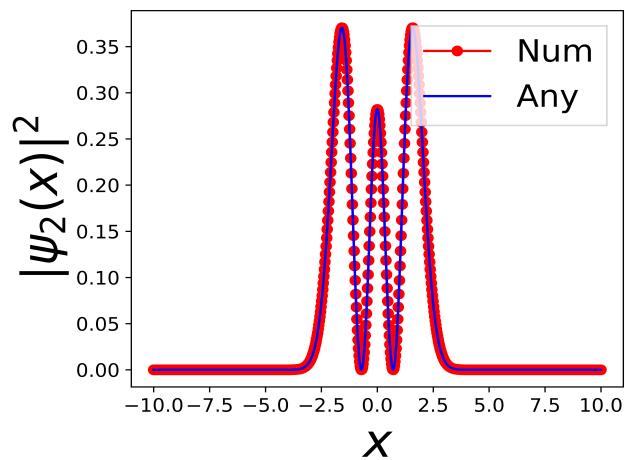


Figure 3.7: Numerical and Analytical plots of probability of Harmonic Oscillator for $n=2$

In fig 3.5 we have one peak which shows that probability of finding particle is maximum at center and decreases as we go away from center. In fig 3.6 we have two peaks having probability maximum at those two points and zero at center region. Same scenario in fig 3.7 but here we have three peaks, two with maximum probability and one with more than half probability in center region.

3.4 Physical Significance of Quantum mechanical Harmonic oscillator

The significance of quantum harmonic oscillator comes from their ubiquity, they are absolutely everywhere in physics. We could spend an enormous amount of time trying to understand why this is so?

So let us study few significances of harmonic oscillator.

3.4.1 Trapped particles

Imagine a small system in which a particle is trapped in a quadratic potential. If the system is sufficiently small, then quantum effects will dominate, and the quantum harmonic oscillator will be needed to accurately describe its dynamics.

3.4.2 Quantum fields

This is perhaps the most fundamental and important item of the lists. It turns out that the most fundamental physical model we currently have, namely the Standard Model of particle physics, is ultimately based on quantizing classical fields (like electromagnetic fields) and realizing that particles basically just emerge from excitations of these fields, and these excitations are mathematically modeled as an infinite system of coupled, quantum harmonic oscillators [6] .

3.4.3 Approximation of Morse potential

The quantum harmonic oscillator is the quantum analog of the classical harmonic oscillator and is one of the most important model systems in quantum mechanics. This is due in partially to the fact that an arbitrary potential curve $V(x)$ can usually be approximated as a harmonic potential at the vicinity of a stable equilibrium point. Furthermore, it is one of the few quantum-mechanical systems for which an exact, analytical solution exists. Solving other potentials typically require either approximations or numerical approaches to identify the corresponding eigenstates and eigenvalues.

Almost all diatomics like H_2 O_2 N_2 F_2 have potentials V , experimentally determined for their lowest energy states i.e $n < 10$. When we go to higher energy states, it is difficult to calculate energy of diatomic bond because now in higher energy states the potential is actually Morse potential. Morse potential, named after physicist Philip M. Morse, is a shadow for the vibrational structure of the molecule than the harmonic oscillator because it explicitly includes the effects of bond breaking and accounts for the anharmonicity of real bonds.

In order to find Dissociation energies of bond in higher states, we approximate Morse potential to Harmonic Oscillator by neglecting higher order terms of eq 3.43

$$V(x) = V(x_o) + \frac{dV(x)}{dx} \Big|_{x_o}^x (x - x_o) + \frac{1}{2!} \frac{d^2V(x)}{dx^2} \Big|_{x_o}^x (x - x_o)^2 + \dots \frac{1}{n!} \frac{d^nV(x)}{dx^n} \Big|_{x_o}^x (x - x_o)^n \quad (3.43)$$

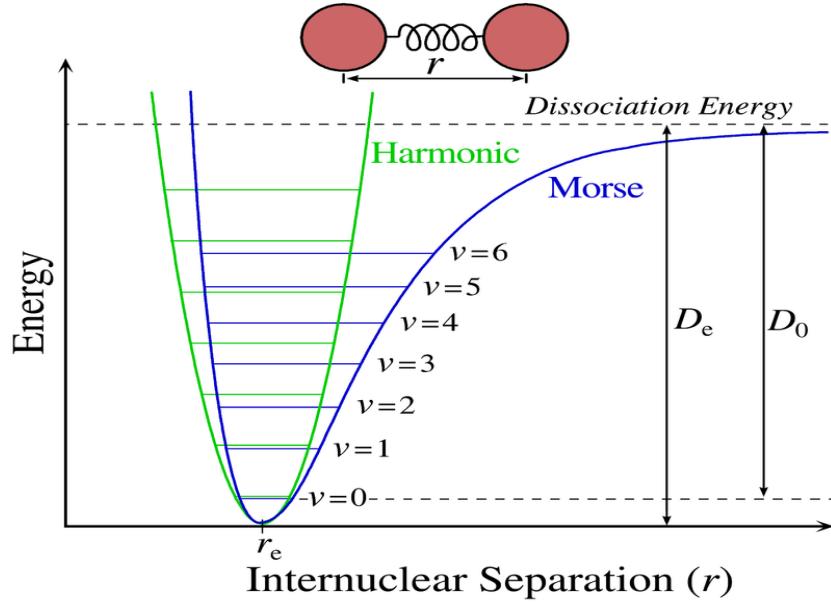


Figure 3.8: The Morse potential (blue) and harmonic oscillator potential (green). Unlike the energy levels of the harmonic oscillator potential, which are evenly spaced by $\hbar\omega$, the Morse potential level spacing decreases as the energy approaches the dissociation energy.

Chapter 4

Double-well Potential

Double-well potentials are important class of configurations which have been extensively used in many fields of physics and chemistry for description of motion of a particle under two centers for force. Recently, solutions of Schrödinger equation with double-well potentials have found applications in the Bose-Einstein condensation, molecular systems, quantum tunneling effect, semiconductors, and so forth [3] .

The double-well potential is arguably one of the most important potentials in quantum mechanics, because the solution contains the notion of a state as a linear superposition of ‘classical states, a concept which has become very important in quantum information theory. It is therefore desirable to have solutions to simple double well potentials [5] .

4.1 Numerical Method

Just like Infinite-Square well and Harmonic Oscillator, again we used Finite-Difference method to plot our wavrfuctions. First step in this method is to to define a step potential that creates our double well.

4.1.1 Unit step Function

“A function that increases or decreases abruptly from one constant value to another.” This is also known as Heaviside funbtion. This function is defined by,

$$H(x) = \begin{cases} 0, & \text{for } x < 0 \\ 1, & \text{for } x \geq 0 \end{cases}$$

Simple step function is shown in fig 4.1,

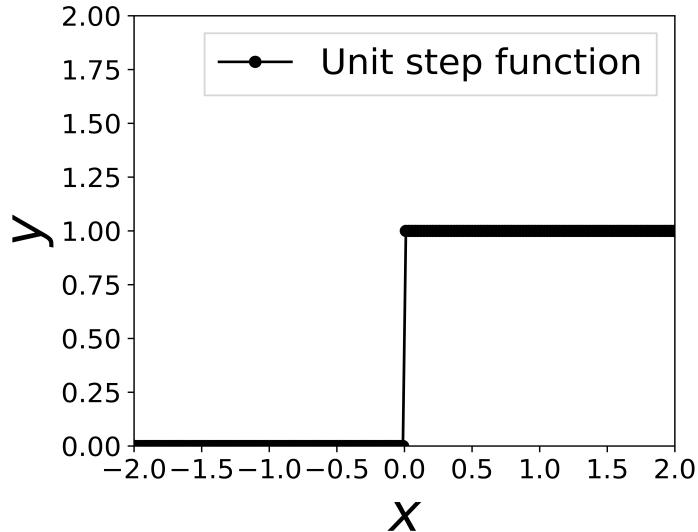


Figure 4.1: Unit Step Function

Using this function in python, we created double-well potential. After defining step function, define the points at which the function changes and the magnitude of step functions known as potential that are V_D and V_m .

In fig 4.2 we have 5 regions, in region 1 and 5 we have very high potential at boundaries i.e $V_D = 1000$. similarly, in region 2 and 4 we have zero potential with $V_m = 80$ is the potential in region between x_1 and x_2 , so two wells are formed. $x_1 = 0.2$ and $x_2 = 1.2$ are points that shifts our step function to make double well potential.

$$V(x) = V_D * \text{step_func}(x - x_2) + V_m * \text{step_func}(x + x_1) - V_m * \text{step_func}(x - x_1) + V_D * \text{step_func}(-x - x_2) \quad (4.1)$$

This function makes our double well potential that is shown in fig 4.2, after creating double well potential, we use finite-difference method to solve Laplacian. Hamiltonian is created after Laplacian and we get eigen energies and corresponding eigen vectors.

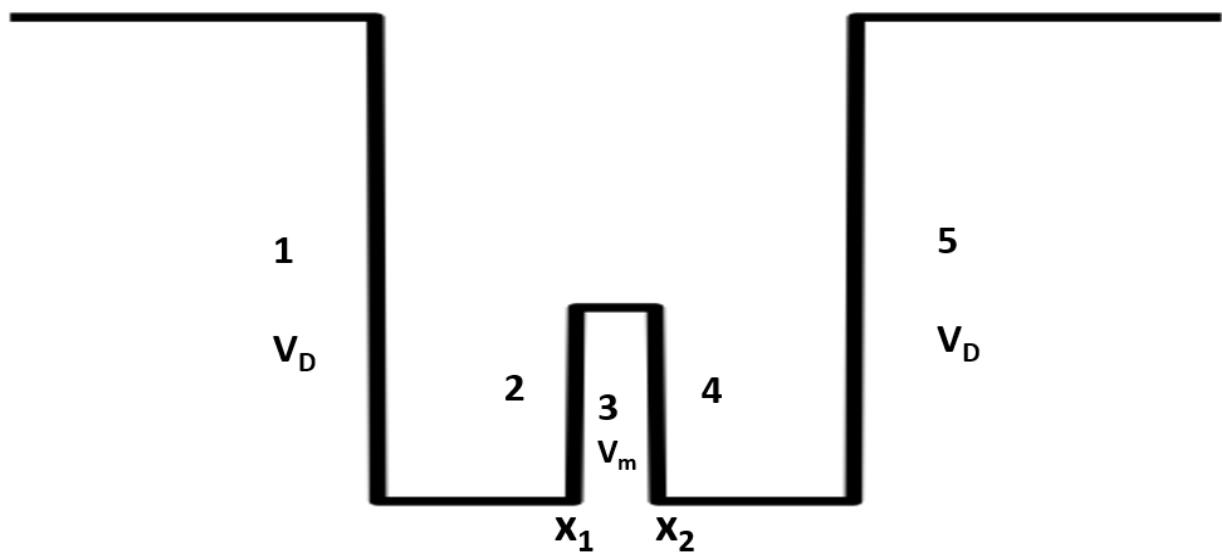


Figure 4.2: Double-well

4.2 Conclusion

After solving Numerically, we plot the wavefunctions and probabailities of particle in double well potential.

Wavefunctions

Plotting first three energy wavefunctions for particle in double well potential.

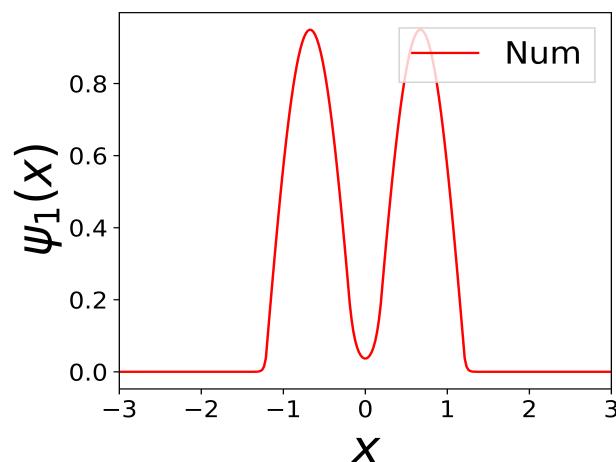


Figure 4.3: Wavefunction Numerical plot of Double-well potential for n=1

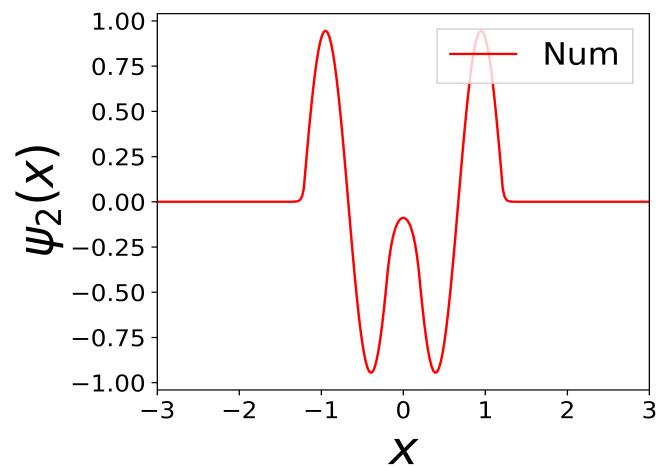


Figure 4.4: Wavefunction Numerical plot of Double-well potential for n=2

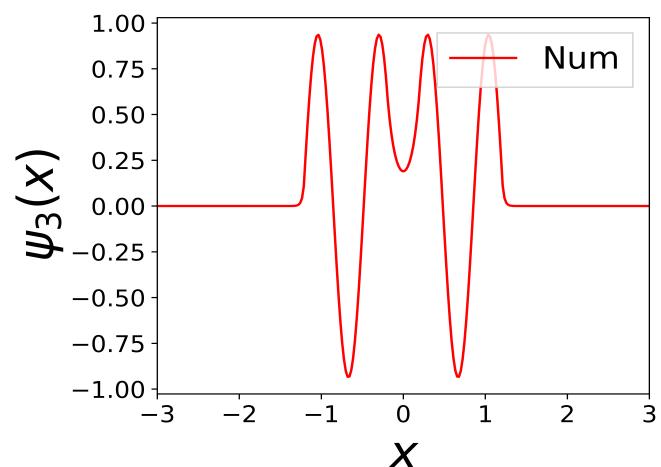


Figure 4.5: Wavefunction Numerical plot of Double-well potential for n=3

fig 4.3 show the numerically plotted wavefunction for ground state. Fig 4.4 shows wavefunction for n=2 and similarly fig 4.5 shows wavefunction for n=3.

Probabilities

After plotting numerical wavefunctions, we plot probabilities of particle in first three energy states of Double-well potential.

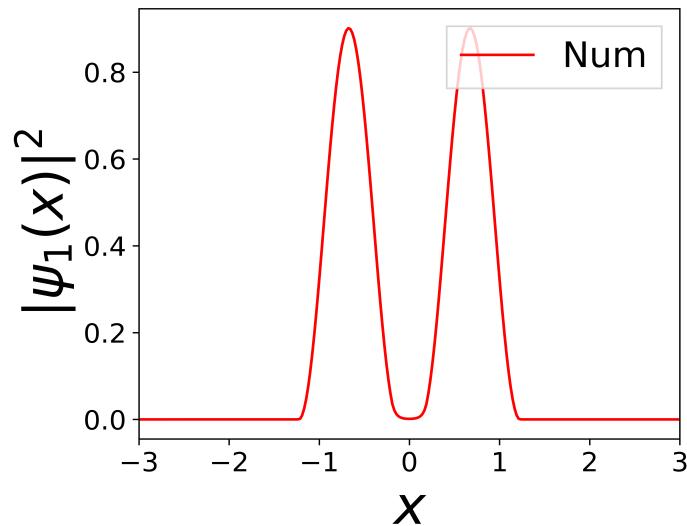


Figure 4.6: Probability Numerical plot of Double-well potential for n=1

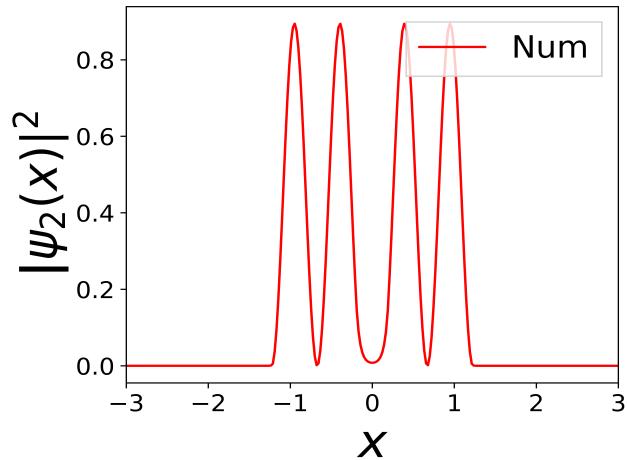


Figure 4.7: Probability Numerical plot of Double-well potential for $n=2$

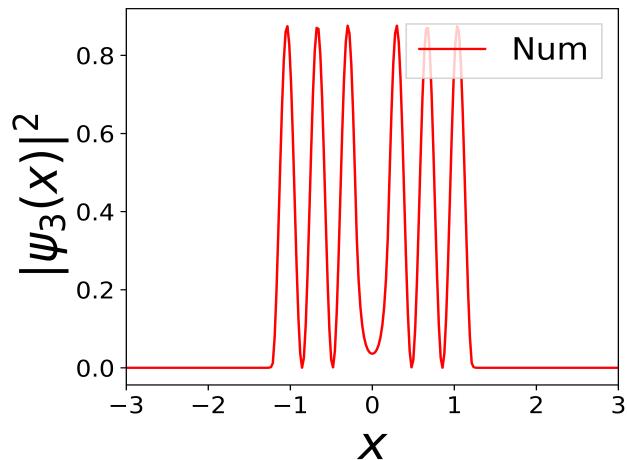


Figure 4.8: Probability Numerical plot of Double-well potential for $n=3$

In fig 4.6 we can see that the probability of finding particle in left and right region is zero because of very high potential at the end regions. Similarly, in fig 4.7 and 4.8 we again have same situation that having zero probability of finding particle at ends and also in middle because we also have potential in middle but have low value as compared to boundaries region.

4.3 Physical significance of Double-well potential

The progress of semiconductor fabrication technology has changed that, as we are now able to make artificial systems of square potential energy wells. Semiconductor quantum wells are now routinely used to fabricate diode lasers and other semiconductor devices. The key advance that allowed fabrication of quantum well devices was the ability to grow pure crystals of semiconductors using techniques such as molecular beam epitaxy (MBE) and metalorganic chemical vapor deposition (MOCVD). With these techniques, layers of semiconductors can be grown with atomic scale precision, yielding structures with layers thin enough (several nm or less) for quantum effects to be important [7] .

4.3.1 Semiconductors

When a material with lower bandgap energy is sandwiched between the material having higher bandgap energy it behaves as Double-well potential. In semiconductors, we deal with different materials, let we have an example of AlAs, AlGaAs and GaAs.

When electrons passes from AlGaAs they face lot of resistance because of high band gap of this semiconductor but GaAs allows electron to pass easily from them, such that no resistance, again when electrons passes from AlAs, they face resistance again but lower as compared to AlGaAs.

This scenario looks like finite potential well, having high potential in boundaries but low potential in between region.

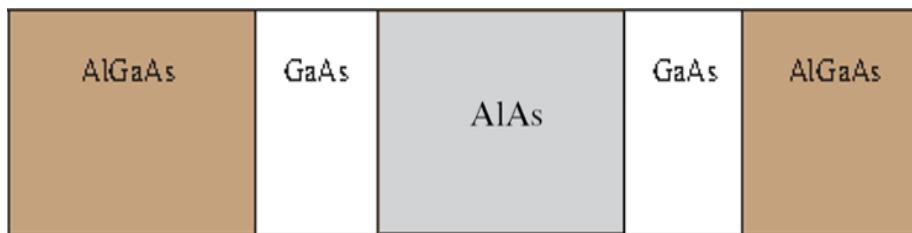


Figure 4.9: AlAs is sandwiched between AlGaAs and GaAs to form double-well potential

Chapter 5

Conclusion

In this thesis, we studied wavefunctions and probabilities of particle in potential wells. Time-Independent Schrödinger wave equation solved for three quantum mechanical potential that are,

- 1. Infinite-Square well**
- 2. Harmonic Oscillator**
- 3. Double-well potential.**

We solved these quantum potentials by using Analytical method that is done by solving Time-Independent Schrödinger wave equation manually and also by Numerical method that is done by using Finite-difference method. To solve these systems, a programming language "Python" is used that gives results precisely and more efficiently.

At first we solved Infinite-Square well potential analytically. Eigen energies, eigen vectors are found to plot wavefunctions and probabilities. After analytical solutions, wave functions and probabilities plotted numerically using finite-difference method. We plotted data for first three energy states. We found that our numerical plots matches quite well with analytical plots of wavefunctions and probabilities of particle in this potential.

Only data in physics is not enough. Understanding the physical meaning of each term is also important. We also studied the physical significance of Infinite-Square well. We studied the real life example of Infinite-square well that is Graphene Quantum Dots that are collections of artificial atoms whose electronic degrees of freedom are quantized. In a semiconductor, these artificial atoms are small boxes of size ranging from 1 nm to 100 nm, capable of holding number of electrons that can be varied as required by varying the number of electrons in the artificial atoms of a semiconductor. That means Quantum dots and Quantum wires can be modeled as Infinite square well.

After Infinite-Square well we studied Harmonic Oscillator. We calculated eigen energies and plotted wave functions and probabilities of particle in Harmonic Oscillator analytically. After analytical solution we solved Time-Independent Schrödinger wave equation numerically using finite-difference method again. We found eigen energies, eigen vectors and plotted wavefunctions and probabilities for first three energy states. We found that our both methods having

same output. We also studied that the major significance of Harmonic oscillator is approximation of Morse well for Diatomic having high potential V. Harmonic oscillator have exact, analytical solution exists. Solving other potentials typically require either approximations or numerical approaches to identify the corresponding eigenstates and eigenvalues. So we approximate Morse potential to get dissociation energy of strong bonds.

In the end we studied Double-well potential. Again we solved Time-Independent Schrödinger wave equation analytically and found eigen energies and wavefunctions. We solved double-well numerically using python and found eigen energies, eigen vectors. We plotted wavefunctions and probabilities for first three energy states and found same results as we found for the analytical method. After all significance of Double-well potential was also studied in detail. We studied that in Semiconductor World we mostly play with materials having high bandgap energies. Double-well potentials formed when low bandgap energy semiconductor sandwiched between very high bandgap material. So electrons flow in material with resistance.

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