# ES202 Project Report

# Numerical Analysis of Schrödinger Wave Equation


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# Problem Statement

The Schrödinger equation is one of the most well known and widely studied equations in physics, having a fundamental role in the field of quantum physics. It is a linear partial differential equation governing the wave function of a quantum mechanical system. In this project, we attempt to solve for the eigenfunctions and eigenvalues of the Schrödinger equation associated with a 1-D quantum well. Specifically, we numerically solved the time independent equations for a “particle in a box” scenario under the conditions of the Infinite, Finite and Inverse $\cosh^2$ potentials. Additionally, we verified the correctness of our solutions by comparing with the analytical solutions and plotting relevant graphs.

# Physical Model

In our everyday lives, we encounter many objects. These objects can be seen and studied by the regular laws of physics. On drastically reducing the size of particles, we enter a very fascinating field of study known as the Quantum realm. The study of behavior of particles in the quantum world is known as Quantum Physics.
The state of the particle in the quantum world is described by the $\Psi(x, y, z, t)$ function. The Schrodinger equation governs the time evolution of the wave function of a system. A one dimensional Schrodinger equation of a particle whose whose wave function is given by Ψ(x, t) is given by

$$(\frac{-h^2}{2m})(\frac{\partial^2\Psi(x,t)}{\partial x^2}) + V(x,t)\Psi(x,t) = i\hbar(\frac{\partial\Psi(x,t)}{\partial t}) \tag{2.1}$$

Our inspiration were waves in the periodical crystal structure of the semiconductors. If an electron enters the periodic crystal, it is going to see electron cloud along its path. This electron tends to move within the crystal in accordance with the lattice potential. In semiconductors, this makes the material conductive. The Kronig-Penny Model of the potential stands as a suitable start point.

As the potential inside a crystal is assumed to be constant, the equation now condenses into solving a time independent Schrodinger equation.

$$\Psi(x,t) = \psi(x)\phi(t) \tag{2.2}$$

# Assumptions

To make the formulation of concept from the vast scope of the Schrodinger equation, we have considered some assumptions in our mathematical model.

1. We have considered the potential of the crystal structure to be stable. This assumption enabled us to come up with the time independent Schrodinger equation.

2. We have assumed that the travelling electron does not have the influence of any other electron, bounded or free, on it.

# Infinite Square Well

## 4.1 Introduction

Here we analyse the time independent infinite square well scenario, which is the most simplified version of the particle in a box problem. It describes the wave function of a particle (e.g. an electron) trapped inside barriers with infinite potential. Unlike the classical case, here the particle can only be present in some specific energy levels, which we intend to find out. Also, its position can vary according to the energy level, and there are even some positions called nodes, where its presence is prohibited.

The time independent version of the Schrödinger equation is given as:

$$(-h^2/2m)\frac{d^2\psi}{dx^2} + V(x)\psi = E\psi \tag{4.1}$$

The eigenvalue equations for this is:

$$H\psi = E\psi \tag{4.2}$$

Where, H is the Hamiltonian Operator $H = (-h^2/2m)\nabla + V(x)$
For the infinite well:

$$V(x) = 0\; for\; L/2 < x < +L/2 \tag{4.3}$$

$$V(x) = \infty\; elsewhere \tag{4.4}$$

For simplicity, we let $(-h^2/2m) = 1$ which gives us:

$$\frac{d^2\psi}{dx^2} = -E\psi \tag{4.5}$$

With boundary conditions as:

$$\psi(\frac{-L}{2}) = 0, \psi(\frac{+L}{2}) = 0, E > 0 \tag{4.6}$$

## 4.2 Analytical Solution

For the analytical solution, we introduce the substitution $k^2 = E$, which makes our equation is:

$$\frac{d^2\psi}{dx^2} = -k^2\psi \tag{4.7}$$

It has a solution that is a superposition of planar waves:

$$\psi(x) = Ae^{i(kx)} + Be^{-i(kx)} \tag{4.8}$$

Now, considering the boundary conditions:

$$\psi(\frac{L}{2}) = Ae^{ik\frac{L}{2}} + Be^{ik\frac{-L}{2}} \tag{4.9}$$

Substituting Cos and Sin functions, in the above equation we get:

$$2[Acos(k\frac{L}{2})] + Bcos(k\frac{L}{2}) = 0 \tag{4.10}$$

$$2i[Ccos(k\frac{L}{2})] - Bcos(k\frac{L}{2}) = 0 \tag{4.11}$$

These two equations will have non-trivial solutions for: A=B

$$Cos(k\frac{L}{2}) = 0 \tag{4.12}$$

Therefore:

$$k_n = (2n+1)\frac{\pi}{L} \tag{4.13}$$

$$\psi(x) = 2ACos(k_n x) \tag{4.14}$$

Symmetrical 'even' Eigenfunction. Similarly, for: B = A

$$Sin(k\frac{L}{2}) = 0 \tag{4.15}$$

Hence:

$$k_n = (2n)\frac{\pi}{L} \tag{4.16}$$

$$\psi(x) = 2ASin(k_n x) \tag{4.17}$$

Symmetrical 'odd' Eigenfunction. Hence, the Eigen-energy can be obtained analytically as:

$$E(n) = \frac{(n^2\pi^2)}{L^2} \tag{4.18}$$

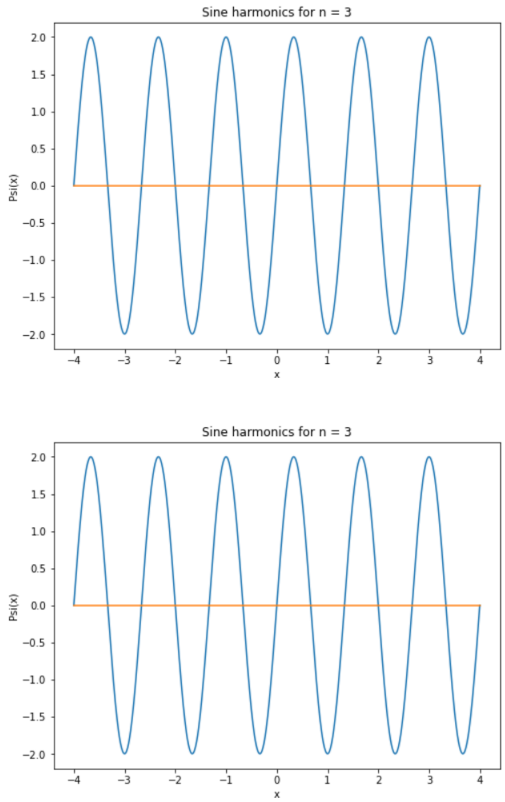


Figure 4.1: Plots corresponding to different eigen-energies (Analytical)

## 4.3 Numerical Solution

We have the equation:

$$\frac{d^2\psi}{dx^2} = -E\psi \tag{4.19}$$

With boundary conditions as:

$$\psi(\frac{-L}{2}) = 0, \psi(\frac{+L}{2}) = 0, E > 0 \tag{4.20}$$

$$let \ \ z = \frac{d\psi}{dx} \tag{4.21}$$

$$=> \frac{dz}{dx} = -E\psi \tag{4.22}$$

Let us consider $x = 0$. Since we know that our solutions are symmetrical, we can break down our initial conditions as either even (i.e. cos) or odd (i.e. sine).
cos conditions:

$$\psi(0) = 1, \frac{d\psi(0)}{dx} = 0 \tag{4.23}$$

sin conditions:

$$\psi(0) = 0, \frac{d\psi(0)}{dx} = 1 \tag{4.24}$$

Given the differential equation and initial conditions, we need to find the different Eigen-energies that satisfy them. We use the Shooting Method for the same.
Let us consider the cos conditions. First, we guess a value for $E$, which we put into the Runga-Kutta function along with cos initial conditions. The obtained value must satisfy the boundary conditions for $\psi(L/2) = 0$. If the values don't match, we need to adjust our guess value of $E$, which we can do using the Bisection method with some degree of error. We continue this to find different values of $E$ which will be our eigen-energies for different $n$.
We observed that the results from analytical and numerical values match almost.

## 4.4 Results and Analysis

| n | E (Numerical) | E (Analytic) |
|---|---|---|
| 1 | 0.6168503761291504 | 0.6168502752 |
| 2 | 2.4674015045166016 | 2.467401101 |
| 3 | 5.551654815673828 | 5.551652477 |
| 4 | 9.869606018066406 | 9.869604404 |
| 5 | 15.421249389648438 | 15.42125688 |
| 6 | 22.206619262695312 | 22.20660991 |
| 7 | 30.225662231445312 | 30.22566349 |
| 8 | 39.478424072265625 | 39.47841761 |
| 9 | 49.964874267578125 | 49.96487229 |

Table 4.1: Comparison between the Numerical and Analytical solutions

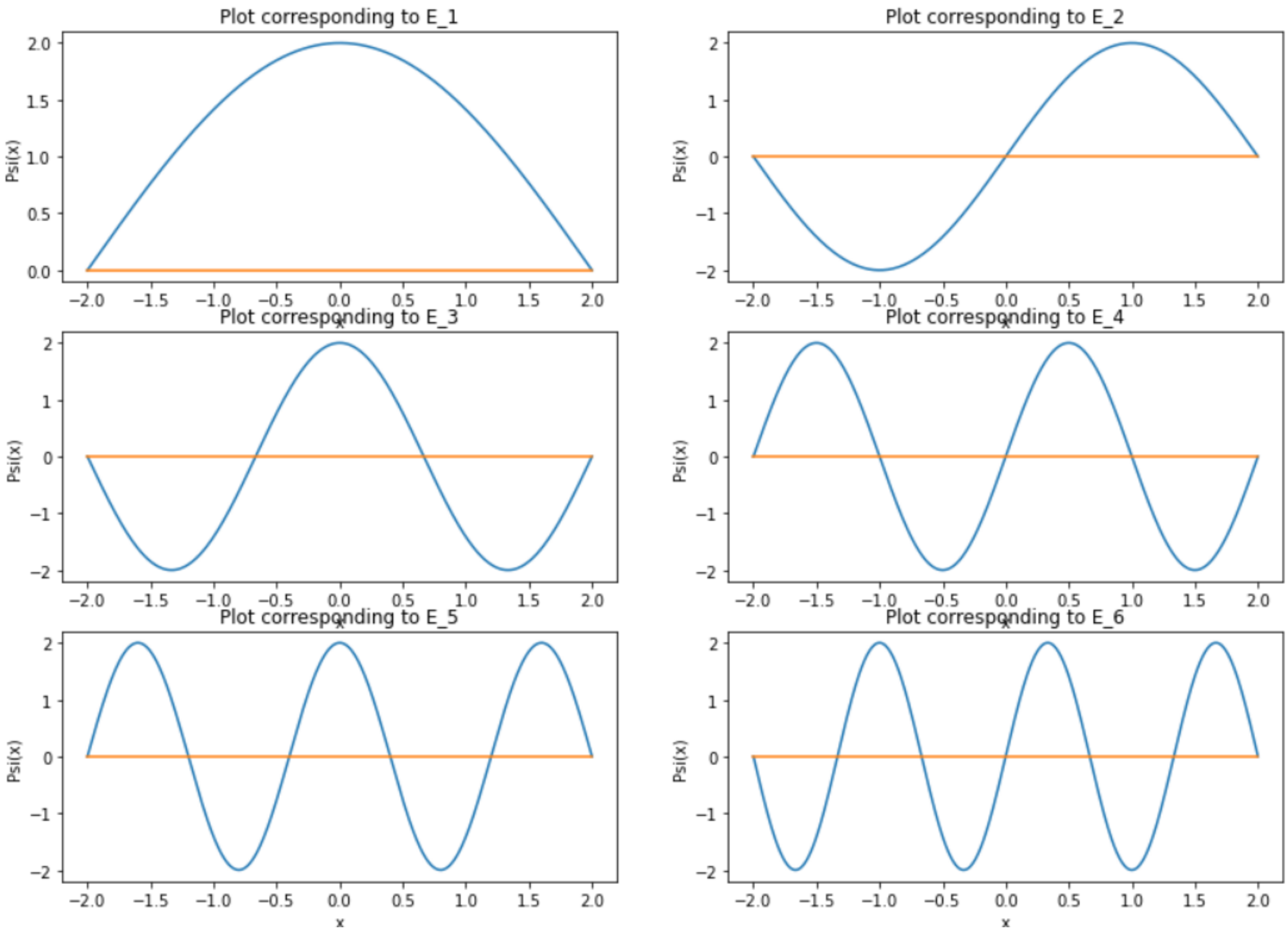


Figure 4.2: Plots corresponding to different eigen-energies (Numerical)

# Finite Square Well

## 5.1 Introduction

Now we are going to increase our numeral solution to a more innovative and complicated process, i.e Finite potential well.

$$V(x) = 0, x > \frac{L}{2}, x < \frac{-L}{2} \tag{5.1}$$

And within these limits:

$$V(x) = -V, \frac{L}{2} > x > \frac{-L}{2} \tag{5.2}$$

So, for the above assignments the Schrodinger Equation is:

$$(\frac{d^2\psi}{dx^2}) = (-E + V)\psi \tag{5.3}$$

## 5.2 Numerical Solution:

### 5.2.1 Wave Functions:

The general solutions of the above Schrodinger Equation are the following wave functions;

$$\psi(x) = a_1 e^{(kx)} + b_1 e^{(-kx)} for x < \frac{-L}{2} \tag{5.4}$$

$$\psi(x) = a_2 e^{(kx)} + b_2 e^{(-kx)} for \frac{-L}{2} < x < \frac{-L}{2} \tag{5.5}$$

$$\psi(x) = a_3 e^{(kx)} + b_3 e^{(-kx)} for x < \frac{L}{2} \tag{5.6}$$

Where the constants K, and , are given by:

$$K = \sqrt{(-|E| + V)} \tag{5.7}$$

$$K = \sqrt{(|E|} \tag{5.8}$$

According to Schrodinger wave, the $\psi(x)$ should be continuous and differntiable everywhere, so when $x \to \pm$. Hence $b1 = a3 = 0$. Due to symmetry nature of the particle motion we will get Even and odd harmonics when we are considering x is changing in -L/2 to L/2

$$\psi(x) = a_1 e^{(kx)} \tag{5.9}$$

$$\psi(x) = a_2 Cos(kx) \tag{5.10}$$

$$\psi(x) = a_1 e^{(-kx)} \tag{5.11}$$

and odd solutions of the form:

$$\psi(x) = -A_1 e^{(kx)} \tag{5.12}$$

$$\psi(x) = A_2 Cos(kx) \tag{5.13}$$

$$\psi(x) = A_1 e^{(-kx)} \tag{5.14}$$

### 5.2.2 Shooting method:

At each and every boundary, the $\psi$ wave function and its derivative, $\frac{d\psi}{dx}$ should be continuous. Therefore, at the right boundary condition (for even functions, for example): So from the continuity perspective

$$a_2 Cos(K(\frac{L}{2})) = a_1 e^{(-k(\frac{L}{2}))} \tag{5.15}$$

From the derivative perspective

$$-Ka_2 sin(K(\frac{L}{2})) = -ka_1 e^{(-k(\frac{L}{2}))} \tag{5.16}$$

$$\frac{d\psi(\frac{L}{2})}{dx} = -k\psi(\frac{L}{2}) \tag{5.17}$$

and Hence this give a simple boundary condition that can be inserted into our present infinite square well code along with the initial conditions, that still apply.

$$\frac{d\psi(\frac{L}{2})}{dx} + k\psi(\frac{L}{2}) = 0 \tag{5.18}$$

Governing equations for Finite square well problem for Schrodinger wave equation

$$\frac{d^2\psi}{dx^2} = (-E + V)\psi \tag{5.19}$$

$$Let \quad z = \frac{d\psi}{dx} \tag{5.20}$$

$$\frac{dz}{dx} = -(E + V)\psi \tag{5.21}$$

$$EvenSolns : \psi(0) = 1, \frac{d\psi(0)}{dx} = 0 \tag{5.22}$$

$$OddSolns : \psi(0) = 0, \frac{d\psi(0)}{dx} = 1 \tag{5.23}$$

Now we will give the initial conditions and the governing differential equations to Runga Kutta method to get the both $\psi(\frac{L}{2})$ and its derivative in $\frac{d\psi(\frac{L}{2})}{dx}$ with a predicted E. For that corresponding E we will check whether 5.18 is nearly satisfying, if it satisfies we got the correct Eigen value. Otherwise we have to change the Eigen value, We can use bisection method to change the intervals where Eigen values can lie.

## 5.3 Transcendental Method

we use transcendental method to verify the value that we obtained in the shooting method. On dividing the equations 5.15 and 5.16 we get

$$k = Ktan(Ka) \tag{5.24}$$

(corresponding to the odd solutions, applying the same as we did for even solutions,we will get)

$$k = -Kcot(Ka) \tag{5.25}$$

(From the equivalent odd Boundary Conditions):

$$K = \sqrt{(-|E| + V)} \tag{5.26}$$

$$k = \sqrt{(|E|)} \tag{5.27}$$

We can assume that the substitution of x = Ka, y = ka to find our equations dimensionless, and define:

$$x^2 + y^2 = r^2 = (\frac{L}{2})^2 V \tag{5.28}$$

Therefore we will get, Even Solution:

$$y = xtan(x) \tag{5.29}$$

Odd Solution:

$$y = -xcot(x) \tag{5.30}$$

note that

$$a = \frac{L}{2} \tag{5.31}$$

Now we will solve (5.28 and 5.29) together and (5.28 and 5.30) to get the corresponding x values from the intersection points. Using that x values we can get E values.
we know that

$$x = Ka = K\frac{L}{2} \tag{5.32}$$

$$K = \frac{x}{(\frac{L}{2})} \tag{5.33}$$

Using 5.26 and 5.33 we will get corresponding Eigen values. We verified that results from Transcendental method and Shooting method. Both the results are almost same.

Note that on solving 5.28 and 5.29 with L=4 we get the equation

$$y = x^2(1 + tan^2(x) - 40 \tag{5.34}$$

$$y = x^2(1 + cot^2(X) - 40 \tag{5.35}$$

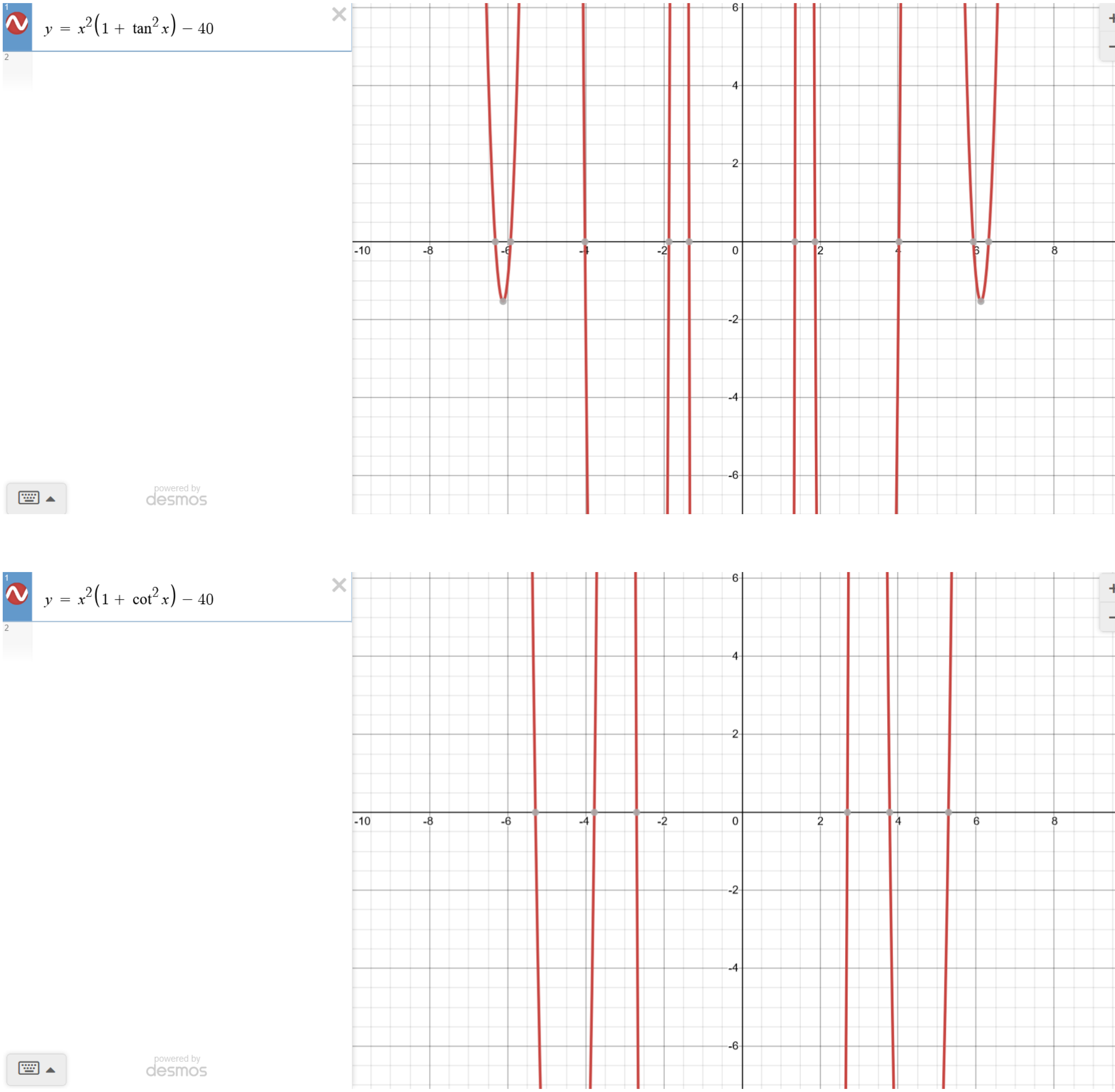

Figure 5.1: Solutions to the transcendental equations corresponding to $tan^2(x)$ and $cot^2(x)$

## 5.4 Results and Analysis

| n | E (Numerical) | E (Analytic) |
|---|---|---|
| 1 | -9.124702972603473 | -9.541069030761719 |
| 2 | -8.176898963974054 | -8.176902770996094 |
| 3 | -5.95393152991528 | -5.953922271728516 |
| 4 | -2.99891663741073 | -2.9989185333251953 |
| 5 | -0.013713849297346314 | 0.013708539307117462 |

Table 5.1: Comparison between the Numerical and Analytical solutions

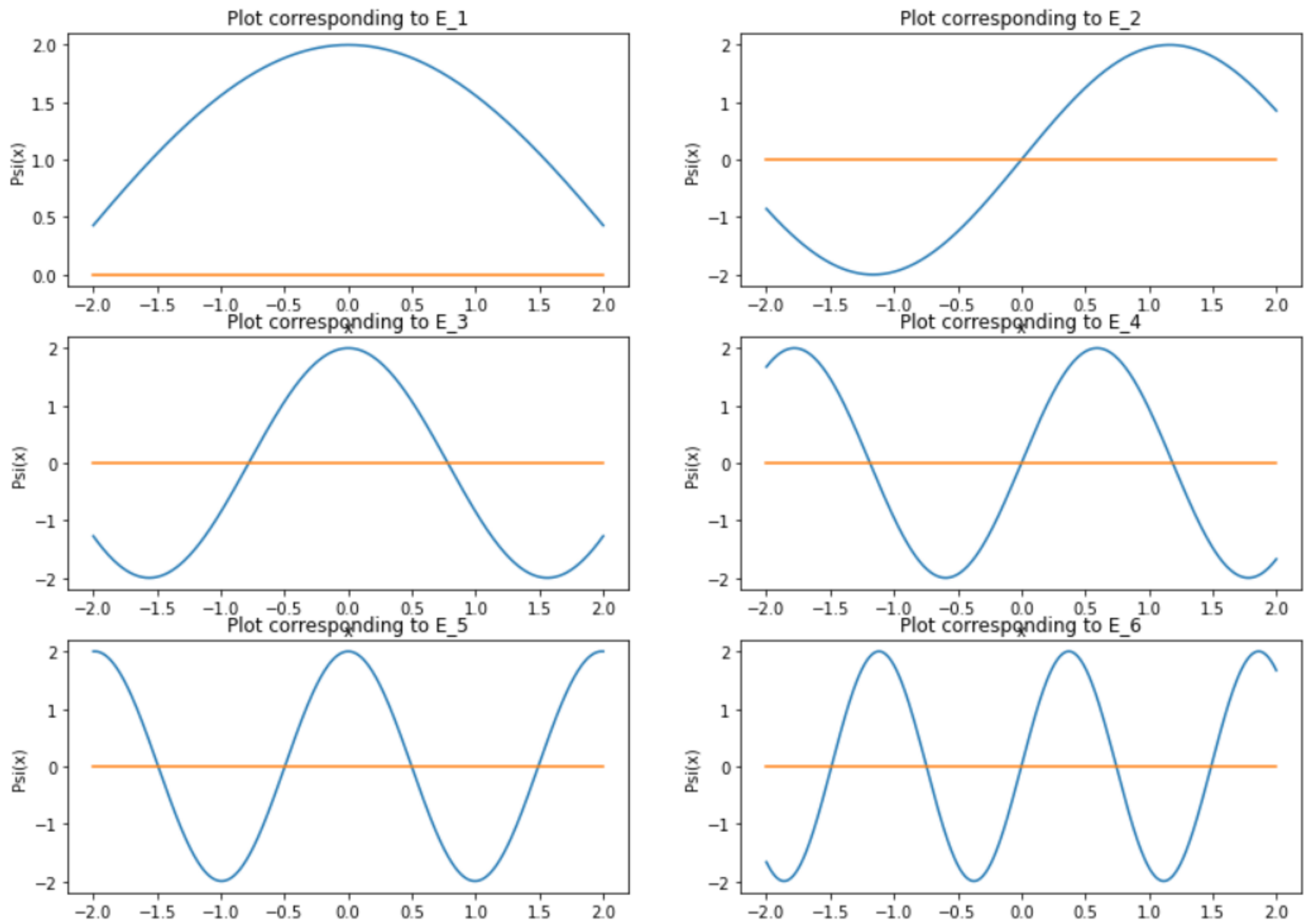


Figure 5.2: Plots corresponding to different eigen-energies inside the well (Numerical)

# Inverse $cosh^2$ Potential

## 6.1 Introduction

A very interesting kind of potential function is the inverse cosh potential. This section deals with numerically approximating the Schrodinger equation when the potential of the one dimensional space is governed by this potential. The potential is described as

$$V(x) = \frac{-V_0}{\cosh^2(\alpha x)} \tag{6.1}$$

And hence, the Schrodinger equation is

$$\frac{d^2\psi}{dx^2} + (E + \frac{V_0}{cosh^2(ax)})\psi = 0 \tag{6.2}$$

This function describes a similar function as the harmonic well having a depth $V_0$ and width scaled by $\alpha$. This function converges to zero as the x converges to positive and negative infinity. Let us consider the following substitution

$$\xi = \tanh(\alpha x) \tag{6.3}$$

This maps the negative infinity of x to -1 and the positive infinity of x to $+1$.

## 6.2 Numerical Approach

The derivatives of (x) in terms of the new variable, are:

$$\frac{d\psi}{dx} = \frac{d\psi}{d\xi}\frac{d\xi}{dx} \tag{6.4}$$

Where..

$$\frac{d\xi}{dx} = \alpha sech^2(\alpha x) \tag{6.5}$$

$$\frac{d\xi}{dx} = \alpha(1 - \xi^2) \tag{6.6}$$

Therefore..

$$\frac{d^2\psi}{dx^2} = \alpha^2(1 - \xi^2)[(1 - \xi^2)(\frac{d^2\psi}{d\xi^2}) - 2\xi(\frac{d\psi}{d\xi})] \tag{6.7}$$

Next, we go to the energy terms of our Schrodinger Equation and make the following substitutions:

$$\epsilon = \sqrt{\frac{-E}{\alpha}} \tag{6.8}$$

and..

$$s(s+1) = \frac{V_0}{\alpha^2} \tag{6.9}$$

$$\frac{d^2\psi}{d\xi^2} = \frac{2\xi}{1-\xi^2}\frac{d\psi}{d\xi} - [\frac{s(s+1)}{1-\xi^2} - \frac{\epsilon^2}{\alpha(1-\xi^2)^2}]\psi \tag{6.10}$$

We define new variables, $\epsilon$ and s for easy solving of the Schrodinger equation.

Let us consider $x = 0$. Since we know that our solutions are symmetrical, we can break down our initial conditions as either even (i.e. cos) or odd (i.e. sine).

cos conditions:

$$\psi(0) = 1, \frac{d\psi(0)}{dx} = 0 \tag{6.11}$$

Sin conditions:

$$\psi(0) = 0, \frac{d\psi(0)}{dx} = 1 \tag{6.12}$$

These initial conditions are the starting point for using the shooting method to figure out the Eigen values of the Energy. We use shooting method to evaluate the boundary condition and verify it, $\psi(1) = 0$. We use the bisection method to navigate the flow of the figured out eigen energy values.

The fourth order Runga-Kutta method is used to estimate the wave function at the required x placements. Although the altered Schrodinger equation is in terms of $\xi$ and $\epsilon$, it is governed by the x and E values.

## 6.3 Analytic Solution

This potential incorporated Schrodinger equation is solved by advanced methods using the Legendre polynomials. This is achieved by using a temporary substitution in the equations. We directly use the results of the analytic method as a base to analyse the numerical approximations.

## 6.4 Results and Analysis

For better scope and analysis, we performed for different values of the minimum potential. We observed that results from the Numerical method almost matches to the values of analytical solution For $V_0 = 10$

| n | E (Numerical) | E (Analytic) |
|---|---|---|
| 1 | -7.298435211181641 | -7.298437881 |
| 2 | -2.8953075408935547 | -2.895313644 |
| 3 | -0.4817233085632324 | -0.4921894064 |

Table 6.1: Comparison between the Numerical and Analytical solutions for $V_0 = 10$

For $V_0 = 15$

| n | E (Numerical) | E (Analytic) |
|---|---|---|
| 1 | -11.594871520996094 | -11.59487516 |
| 2 | -5.784626007080078 | -5.784625486 |
| 3 | -1.9742412567138672 | -1.97437581 |

Table 6.2: Comparison between the Numerical and Analytical solutions for $V_0 = 15$

For $V_0 = 20$

| n | E (Numerical) | E (Analytic) |
|---|---|---|
| 1 | -16.000015258789062 | -16 |
| 2 | -9.000007629394531 | -9 |
| 3 | -3.9999961853027344 | -4 |
| 4 | -0.9967947006225586 | -1 |

Table 6.3: Comparison between the Numerical and Analytical solutions for $V_0 = 20$

The results obtained from the analytical and numerical solutions matches

# References

[1] Wikipedia. 2021 "Finite potential well" Last Modified 18 April 2021.
`https://en.wikipedia.org/wiki/Finite_potential_well`
[2] Wikipedia. 2021 "Schrödinger equation" Last Modified 2 May 2021.
`https://en.wikipedia.org/wiki/Schr%C3%B6dinger_equation`

[3] Neill Lambert, Numerical Solutions of Schrödinger's Equation, April 18, 2001.
https://www1.itp.tu-berlin.de/brandes/public_html/qm/qv3.pdf
[4] Wikipedia. 2021 "Particle in a box" Last Modified 6 May 2021.
https://en.wikipedia.org/wiki/Particle_in_a_box