**Final Project Report PHYS 5319 MM3**

**Solving 1-D Schrödinger equation by the shooting method**

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**Abstract**

The goal of this project is to solve the 1-D Schrödinger equation for a 1-D double-well potential by a numerical shooting method using 4th order Runge-Kutta method. This report contains the analysis of the problem, the methodology used, the python code used, the results, and discussion.

The Schrödinger equation is the fundamental quantum mechanical equation. However, only for a handful of cases it can be solved analytically, thus requiring a numerical method to solve for systems where no analytical solution exists.

The shooting method is a numerical method to solve differential equations such as the Schrödinger equation where the boundary conditions are known and certain parameters to solve the equations must be found. In this project, we study the parameter energy (E) as the eigenvalue of the system. The shooting method used in this project is the double-shooting method. In double-shooting method, we take the left & right boundary conditions as initial conditions of the equation as the starting points and shoot from both left & right side with defined initial values. Then we observe whether the solutions from left & right shooting comes close enough at some matching point. If this is the case, we then refine it further to a specified accuracy.

In this project, the Schrödinger equation is solved for a 1-D double-well potential and later for a simple harmonic oscillator around x0, where x0 is one of the two bottoms of the double-well. To demonstrate the method's accuracy, we use a simple harmonic oscillator around x=0 as a test potential to compare the numerical solutions to their analytical counterparts. Overall, the results match the analytical solutions proving the shooting method to be a useful tool for obtaining numerical solutions for the Schrödinger equation.

**Acknowledgement**

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# Introduction

The goal of this project is to solve the 1-D Schrödinger equation for a 1-D double-well potential by a numerical shooting method using 4th order Runge-Kutta method.

|  |  |
| --- | --- |
|  | (1) |

where the potential *V* is given by,

|  |  |
| --- | --- |
|  | (2) |

with ***a = 2*** and ***b = 8*.**

## Project aims

The motivation for this project is to test out the double shooting method implemented with Python and to see how it can be used for solving the Schrödinger equation. The aims of this project are as following:

1. Find all the energy eigenvalues (E) below zero (E < 0). (at least 4 significant figures)
2. Plot the lowest 2 states (orthonormal wave functions) together with *V(x)* in *(-2.5<x<2.5)*.
3. Discuss that if V(x) is approximated as a simple harmonic oscillator around x0, where x0 is one of the two bottoms, what kind of structures for the energy eigenvalues and wavefunctions will be. Compare (qualitatively) with your results from a) and b).

## Approach

1. Python is a well-suited language for scientific programming with clear, easily readable syntax and add-on packages for many computing needs. This project uses the *NumPy* library and the *matplotlib* plotting environment. It is free and operating system independent, making it easily transferable.
2. The Schrödinger equation takes the form,

|  |  |
| --- | --- |
|  | (3) |

1. The Schrödinger equation takes the form,

|  |  |
| --- | --- |
|  | (3) |
|  |  |

Now this is the standard form of a 2nd order differential equation. Knowing the Schrödinger equation boundary conditions, the solutions for arbitrary energies can be computed with a numerical integration method. The method used here is 4th order Runge-Kutta method. But the issue here is that there is a parameter *E.* Now, here we can use the shooting method which allows us to find both the parameter and the solution of the differential equation.

In this project, double shooting method is used. The idea is to guess the value of *E* and start solving the differential equation using a numerical integration method from both the boundaries (left & right) assuming boundary conditions as the initial values of the function (hence the name double shooting). And the integration will progress till a point (matching point) where we check if the values of the function match. If they match, we keep the values of *E*, else we keep trying different values of *E.* In this way, we will get those values of *E* which will satisfy our differential equation.

The matching energy values can then be refined with either an interpolation method, or with shooting as often as needed.

To test the accuracy of the double shooting method, we use a simple harmonic oscillator around *x = 0* as a test potential to compare the numerical solutions to their analytical counterparts.

# Introduction

## Introduction to the report

## Introduction to my setting

# Literature Review

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