# Quantum Mechanics: Numeric Potential Final Projects

This project will consist of modeling the energy spectrum and wavefunctions of various potential wells, which cannot usually be approached analytically. To complete one of these projects, one should use numerical methods to solve the Schrödinger equation and investigate how the shape and form of different potentials affect the spectrum of bound states. Each problem addresses a different potential and provides insight into different quantum mechanical systems. There are a bunch of potential potential projects listed below, choose one.

## Project Requirements

The final project will be graded based on two main components: a 4-5 minute video presentation and a 5-10 page report. The project should focus on solving for bound states in a specific quantum potential numerically, analyzing the results, and relating them to a real-world experiment or physical system. The following guidelines outline what is expected for each component:

### Video Presentation

- A 4-5 minute video where you present the problem, explain the potential you are using, describe the numerical method for solving for the bound states, and discuss your results.
- Clearly explain the quantum potential (e.g., finite square well, wedge potential, etc.) and how it models a physical quantum system.
- Include a brief discussion on how this quantum potential relates to real-world experiments or technologies (such as semiconductor quantum dots, nuclear potential wells, etc.).

### Report

The report should be 5-10 pages long, written in 12-point font, single-spaced, with 1-inch margins. It should contain the following sections:

- **Introduction:** Provide a brief overview of the quantum potential you have selected (e.g., finite square well, wedge potential, quantum dot) and its significance in quantum mechanics. Explain why understanding bound states in this potential is important for real-world systems.

- **Method:** Describe the numerical method you are using to solve the Schrödinger equation for bound states in the potential. Discuss the numerical techniques (e.g., finite difference, shooting method, etc.) and boundary conditions used.
- **Results:** Present the bound state solutions (energy levels and wavefunctions) you obtained from the numerical method. Provide graphs and visualizations of the bound state wavefunctions and energy levels.
- **Analysis:** Analyze the physical interpretation of your results. Compare the bound state energy levels and wavefunctions to known theoretical predictions (if applicable). Discuss any interesting patterns or features that emerged in the solutions.
- **Applications:** Relate your results to a real-world system or experimental setup, (even/especially of your own devising!). For example, if you are working with the step potential well, you could look into and discuss its relevance to semiconductor materials and the different potentials they will have across material boundaries. You could attempt to use your model to approximate a nuclear well, and relate your results to nuclear physics.

**Numerical Techniques**

- You must include a numerical solution to the Schrödinger equation for your selected potential. This can be done using Python, Mathematica, or another computational tool.
- Your code and results should be included as an appendix or supplementary material.

**Note:** Shorter reports with concise and clear explanations are preferred over longer, less clear reports.

# 1 Finite Parabolic Well

In this project, the potential has a parabolic form with a finite cutoff. It is described as:

$$V(x) = \begin{cases} \frac{1}{2}m\omega^2 x^2 & |x| \leq a \\ V_0 & |x| > a \end{cases}$$

This potential combines features of both a harmonic oscillator and a finite square well, confining the particle within a parabolic well for $|x| \leq a$ and having a finite barrier outside the well.

1. Solve the Schrödinger equation numerically for this finite parabolic well.

2. Compute the bound state energies and wavefunctions for different values of $V_0$, $\omega$, and $a$.
3. Analyze how the finite cutoff in the potential affects the energy levels compared to a pure harmonic oscillator.
4. Discuss a physical system you could construct that would be well-modelled by the finite parabolic well. In what sense would it matter that you'd modelled it as finite parabolic rather than the infinite parabolic well? (One option would be to investigate optical trapping of silicon beads, although you may find literature that the trapping potential isn't strictly harmonic.)

# 2 Multi Part Square Potential

This problem examines a square step potential, which creates a sharp transition between two regions of different potential energy. We might take this as first approximation for the behavior of particles moving between semiconductor regions with different internal properties/potentials. The potential is given by

$$V(x) = \begin{cases} -V_0 - V_1 & -a \leq x \leq 0 \\ -V_0 & 0 \leq x \leq a \\ 0 & |x| > a \end{cases}$$

You are tasked with solving for the bound state energies for this system and associated wavefunctions.

1. Solve the Schrödinger equation for the wavefunction in the bound state region - you will want to implement a numeric solution.
2. Taking $E < 0$, determine for some cases whether bound states exist in this system.
3. Use a numerical method to visualize the wavefunctions and analyze the energy levels for both the scattering and bound states.
4. Relate this to a real-world physical system.

# 3 Quantum Dot Model

In this project, you will model the quantum confinement effects in a quantum dot, where the particle is confined in a finite potential well, surrounded by a more realistic region of lower potential. This is pretty much the same as the Multi Part Square Potential, but now there are three parts with a well at the center. Note that below $|L| > |a|$, and $\alpha$ is a positive constant which determines the depth of the quantum dot.

$$V(x) = \begin{cases} -V_0 - \alpha V_0 & |x| \leq a \\ -V_0 & a \leq |x| \leq L \\ 0 & |x| > L \end{cases}$$

Quantum dots are nanostructures where electrons are confined in a small region of space, leading to discrete energy levels.

1. Numerically compute the energy spectrum and wavefunctions for a particle confined in the quantum dot.

2. Investigate how the energy levels change as the potential depth $\alpha$ and the width $a$ are varied relative to $L$ and $V_0$.

3. Look into how this relates to the behavior of electrons in quantum dots, or find some other physical system to relate this potential to.

# 4 Multiple Well Spectrum

This project examines a system with multiple wells, which creates a more complex potential landscape. The potential consists of a series of wells, modeled as:

$$V(x) = \begin{cases} -V_0 & \text{for regions of size } a \text{ spaced apart by } L\text{, with at least 2 such wells} \\ 0 & \text{between wells} \\ \infty & \text{elsewhere} \end{cases}$$

The goal is to compute the energy spectrum and investigate the effects of tunneling between adjacent wells. If you choose to only consider 2 wells, you should also either vary the well widths (2 different well widths) and/or the well depths (2 different well depths.)

1. Use numerical methods to solve for the bound states of a particle confined in this multiple well potential.

2. Analyze how the presence of multiple wells affects the energy levels, particularly in comparison with a single well.

3. Investigate the wavefunction solution for the whole system, and discuss any "tunneling effect" between adjacent wells and how this influences the energy levels.

4. Relate this to a real-world physical system.

## 5 Perturbed Square Well

In this project, you will examine a not-so-square well, where impurities perturb the otherwise clean square well potential. The potential is described by:

$$V(x) = \begin{cases} -V_0 + V_d \exp\left(-\frac{x^2}{\xi_d^2}\right) & |x| \leq a \\ 0 & |x| > a \end{cases}$$

Here, $V_d < V_0$ represents the impurity potential, and $\xi_d$ is the spatial extent of the impurity.

1. Numerically solve for the bound states of the particle in this dirty square well.
2. Investigate how the impurity potential affects the energy levels and wavefunctions.
3. Compare your results with the clean square well and discuss how the presence of impurities modifies the quantum states.
4. Relate this to a real-world physical system.

## 6 Bound State Spectrum

This project investigates a potential that interpolates between a harmonic oscillator and a square well. The potential takes the form:

$$V(x) = |x|^\beta$$

where $\beta \geq 2$. The goal is to explore how the energy spectrum changes as $\beta$ varies.

1. Numerically compute the bound state energies for different values of $\beta$.
2. Investigate how the spacing between energy levels evolves as the potential changes from a square well ($\beta \to \infty$) to a harmonic oscillator ($\beta = 2$).
3. Analyze how the form of the wavefunctions changes as the potential shifts between these two limits.
4. Identify some physical system or experimental setup where the shift from a harmonic oscillator to infinite square well might be physically realized. What would happen to the spectrum of states as this occurred? How would this occur?