Understanding the Shooting Method As Applied to 1D Quantum Potentials
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Learning Objectives

1.) Students will be able to describe the shooting method for solving for eigenvalues and eigenfunctions for the infinite square well.
2.) Students will see that the solution to the 1D Schrodinger equation is insensitive to the choice of initial guess of the slope.
3.) Students will explore the calculated endpoints of each Euler Projection at a given Energy to identify bad solutions and good solutions (Eigenvalues, Eigenfunctions).
4.) Students can evaluate the error from the exact values using the analytical form of the solution to the infinite square well (optional).
5.) Students can implement a computer aided search of the functional to determine the Eigenvalues (optional).

Introduction

The system of Particle in a Box (a.k.a. the Infinite Square Well) is shown in (Figure 1). In this system, a particle of mass, m, is confined to a box of length, a. The Schrödinger Equation that governs this system within the box is given in Eq 1.

$$-\frac{\hbar^2}{2m}\frac{d^2\,\Psi(x)}{dx^2} + V(x)\Psi(x) = E\,\Psi(x) \tag{1}$$

There are well known analytic solutions to this form of the Schrödinger Equation. Of relevance here is the energy of each quantum state (n), which is related to $\hbar$ and the mass of the particle, m:

$$E_n = -\frac{n^2\pi^2\hbar^2}{2ma^2}. \tag{2}$$

Obtaining this solution ordinarily requires a knowledge of advanced math concepts including trigonometry and calculus. But it is possible to reduce the solution of the Schrödinger Equation (Eq 1) to simple arithmetic and slopes using the Shooting Method in concert with Euler's Method. A detailed description of this process is available in Ref **?** and will only be summarized here. It is important to note that the Schrödinger Equation is especially amenable to this treatment because there is no explicit dependence upon the first derivative of the wave function.

Euler's Method (Figure 2) reduces the solution of a first order differential equation to the calculation of a number of linear steps of width, dX assuming one knows the initial value of a the function. Mathematically, this results in a recursion formula to calculate the next point $(i+1)$ from the previous point (i).

$$y_{i+1} = y_i + dX\,y_i'\,;\,y_0 = Y0 \tag{3}$$

The first derivative, y_i' is just $\frac{\Delta y_i}{\Delta x_i}$. This formulation reduces the calculus to simple addition and multiplication.

The Schrödinger Equation for Particle in a Box is a Boundary Value Problem. A Boundary value problem is a differential equation where the solutions are fixed by constraints at the boundary of the problem. Here, the boundary conditions require that the wavefunction $\Psi(x)$ goes to 0 at the both ends of the box. The Euler Method though allows one to solve an Initial

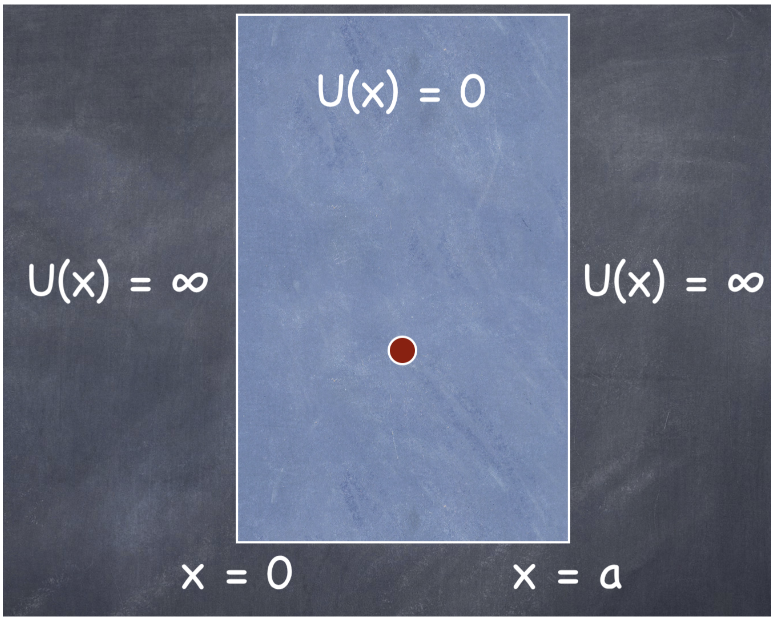

Figure 1: The Infinite Square Well. A particle of mass m is confined to a box where the potential U(x) inside the box is 0 and outside the box is infinite. This leads to a quantized system with well-defined energy levels. The allowed energy transitions change as the mass of the particle is varied in a box of fixed length, a.

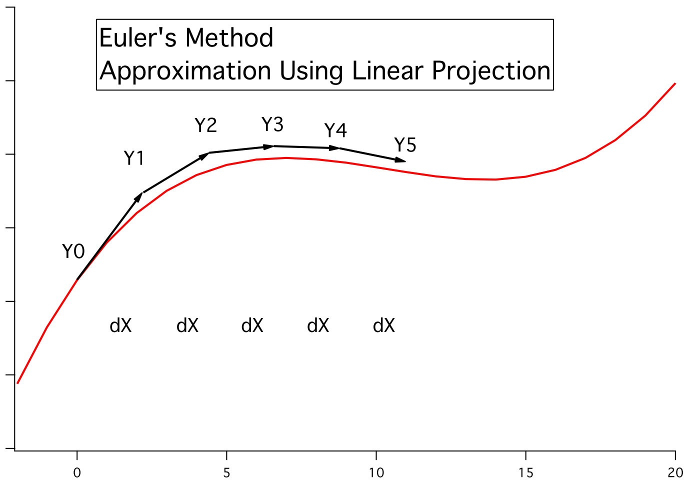

Figure 2: Euler's Method allows one to approximate a curve as a series of linear projections where the differential equation is just used to determine the slope of the tangent line (m $= \frac{\Delta y}{\Delta x}$) at at given point.

Value Problem. Initial value problems are differential Equation where the solutions are fixed by the initial value and slope of the unknown function. The Shooting Method provides a simple bridge from an initial value problem to a boundary value problem.

In the Shooting Method, we have to guess at the initial values of the slope which when propagated will take us to the required boundary value ($\Psi(a) = 0$). The interesting feature of the Schrödinger Equation for Particle in a Box is that there is no dependence upon the slope. Any value that we guess for the initial slope can potentially give a valid answer, excluding the normalization which can be taken care of after the fact. The Shooting Method compares the prediction at the boundary to the expected value in order to determine the values of of the E_n. The Shooting Method for Particle in a Box requires one to find the condition where:

$$abs(\Psi(a)_{calc} - \Psi(a)_{actual}) < \epsilon. \tag{4}$$

For a particle in an infinite square well, $\Psi(a)_{actual} = 0$. Students must vary the assumed energy until the criteria above is reached. For Particle in a Box, the two Euler Equations are as follows:

$$\Psi_{i+1} = \Psi_i + \Psi_i' * dx; \tag{5}$$

and

$$\Psi_{i+1}' = \Psi_i' + \frac{2\,m\,(V_i - E_{guess})}{\hbar^2}\,\Psi_i * dx \tag{6}$$

where the primed variables are derivatives with respect to x.

Exercises

1.) Have the student identify the first few eigenvalues of the Infinite Square Well by running the program with different energy windows. If they would like they can use Eq 2 to predict the windows.
2.) Have the students pay particular attention to the direction from which the improper solutions approach the eigenvalues. Ask the students to predict from which direction that the solution will be approached for the next eigenvalue.
3.) Have the students demonstrate that the eigenvalues and eigenfunctions are not sensitive to the initial guess of the slope. Have them explain why (or why not) that this should be the case.
4.) Have the students calculate the error from the exact solution for a 10 Å box using Eq 2.
5.) Have the students implement a root finder for the functional.