Numerical Solution of the One-Dimensional Schrödinger Equation

Project Summary
In this project, I numerically solved the one-dimensional time-independent Schrödinger equation (TISE) to study the quantized energy spectrum and stationary states of a quantum particle confined in a potential. Since most quantum systems do not admit analytical solutions, this project focuses on understanding how numerical methods can be used to solve quantum mechanical eigenvalue problems.

Physical Background
In quantum mechanics, the state of a particle is described by a wavefunction $\psi(x)$, whose squared magnitude $|\psi(x)|^2$ represents the probability density of finding the particle at position x. The allowed energy states of the system are obtained by solving the time-independent Schrödinger equation

-(hbar^2 / 2m) d^2ψ(x)/dx^2 + V(x)ψ(x) = Eψ(x),

where V(x) is the potential energy and E denotes the energy eigenvalue. This equation can be written in operator form as $H\psi = E\psi$, where H is the Hamiltonian operator. This shows that determining the allowed energies of a quantum system is fundamentally an eigenvalue problem.

Model System
As a test case, I considered a particle in a one-dimensional infinite potential well of length L. Inside the box, the potential is zero, while it is infinite outside, enforcing boundary conditions $\psi(0)=\psi(L)=0$. Although this system has an exact analytical solution, it serves as an ideal benchmark for validating numerical methods.

Numerical Methodology
The spatial coordinate was discretized into a uniform grid, and the second derivative in the Schrödinger equation was approximated using the finite difference method. This converts the differential equation into a matrix equation, where the Hamiltonian operator becomes a tridiagonal matrix consisting of kinetic and potential energy terms. The resulting matrix eigenvalue problem was solved numerically using standard linear algebra routines to obtain energy eigenvalues and corresponding eigenstates.

Results and Verification
The lowest few energy eigenvalues obtained numerically were compared with the known analytical results for the particle-in-a-box system. The numerical energies were found to converge to the analytical values as the grid resolution increased, confirming the accuracy and stability of the method. The computed eigenfunctions exhibit the expected nodal structure, with higher energy states having an increasing number of nodes.

Significance of the Project
This project demonstrates how quantum mechanical problems can be approached using computational techniques, bridging concepts from quantum physics, numerical analysis, and linear algebra. The same framework can be directly extended to more realistic potentials (such as the harmonic oscillator or finite wells), where analytical solutions are not available. Through this work, I developed a clearer understanding of quantum eigenvalue problems and the role of numerical methods in modern theoretical and computational physics.

One-Line Summary
I numerically solved the one-dimensional time-independent Schrödinger equation by discretizing the Hamiltonian using finite difference methods and obtained energy eigenvalues and eigenstates through matrix diagonalization, verifying the results against analytical solutions.