Numerical Solution of the Time-Independent 1D Schrödinger Equation

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Abstract

0 Keywords & Preliminaries

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1 Background & Theory

In this computational laboratory, we shall be solving the time-independent Schrödinger equation for a particle in a one-dimensional potential well. The time-independent Schrödinger equation is

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

where $\psi(x)$ is the wavefunction of the particle, $V(x)$ the potential the particle is under, m the mass of the particle, E the energy of the particle and $\hbar$ the reduced Planck constant. In this lab, we shall remove the dimensions from this equation, to avoid computation of excessively small numbers. Thus we get the non-dimensional Schrödinger equation.This is given by

$$\frac{\mathrm{d}^2\psi(\tilde{x})}{\mathrm{d}\tilde{x}^2} + \gamma^2(\varepsilon - \nu(\tilde{x}))\psi(\tilde{x}) = 0 \tag{2}$$

where our non dimensional constants, variables and functions are $\tilde{x} = x/L$, $\varepsilon = E/V_0$, $\nu(\tilde{x}) = V(\tilde{x})/V_0$ and

$$\gamma^2 = \frac{2mL^2V_0}{\hbar^2} \tag{3}$$

1.1 Discretization of Wavefunction and its Derivatives

To find a numerical solution for this equation, we first discretize our continuous coordinate $\tilde{x}$ and wavefunction $\psi(\tilde{x})$ into N points. Thus each point is defined by $\tilde{x}_n = \frac{n}{N}$, $n = 0, 1, ..., N$. To discretize our wavefunction, we Taylor expand $\psi(\tilde{x} \pm l), l = 1/(N-1)$ about $\tilde{x}$ up to fourth order, and adding the two expansions giving us

$$\psi(\tilde{x} + l) + \psi(\tilde{x} - l) = 2\psi(\tilde{x}) + l^2\psi''()\tilde{x}) + \frac{l^4\psi^{(4)}(\tilde{x})}{12} + O(l^6) \tag{4}$$

2 Methodology

3 Results

3.1 Analytic Solution of non-dimensional Schrödinger Equation

Our first task is to solve the non-dimensional Schrödinger equation analytically, so that we can later verify our computational results. We must solve for the potential well defined by

$$\nu(\tilde{x}) = \begin{cases} -1 & \text{if } 0 < \tilde{x} < 1 \\ \infty & \text{otherwise} \end{cases} \tag{5}$$

To do this we first write our non-dimensional Schrödinger equation

$$\frac{\mathrm{d}^2\psi(\tilde{x})}{\mathrm{d}\tilde{x}^2} + \gamma^2(\varepsilon + 1)\psi(\tilde{x}) = 0 \tag{6}$$

since ε has no $\tilde{x}$ dependence, the solution is simply

$$\psi(\tilde{x}) = \begin{cases} Ae^{ik\tilde{x}} + Be^{-ik\tilde{x}} & \text{if } x \in (0,1) \\ 0 & \text{otherwise} \end{cases} \tag{7}$$

where $k = \gamma\sqrt{\varepsilon + 1}$. We let $\psi_M(\tilde{x}) = \psi(\tilde{x})$ for $x \in (0,1)$. Then, since ψ must be smooth, we can say $\psi(0) = \psi(1) = 0$. This gives us $A + B = 0$, so $A = -B$. Thus we have

$$\psi_M(\tilde{x}) = A(e^{ik\tilde{x}} - e^{-ik\tilde{x}}) = 2iA\sin(k\tilde{x}) = C\sin(k\tilde{x}). \tag{8}$$

We then use our second boundary condition, at $\tilde{x} = 1$, giving us $\sin(kx) = 0$. This gives us $k_n = n\pi$ for $n \in \mathbb{N}$. To find the solutions we then normalise the wavefunction (integrate $|\psi|^2$ and equate to 1), giving us $C = \sqrt{2}$. Thus we have our analytic solutions

$$\psi_n(\tilde{x}) = \sqrt{2}\sin(n\pi\tilde{x}) \tag{9}$$

from our equivalent k_n definition we solve for our energy values ε_n,

$$\varepsilon_n = \frac{n^2\pi^2}{\gamma^2} - 1 \tag{10}$$