Numerical Solver for Time Independent Schrödinger Equation

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Time Independent Schrodinger Equation

$$-\frac{1}{2}\psi(x) + V(x)\psi(x) = E\psi(x) \tag{1}$$

where $V(x)$ is the potential function

We will be testing a solver using a potential function

$$V(x) = \begin{cases} \infty & x \leq 0, \\ x & x > 0 \end{cases} \tag{2}$$

This forms the resultant differential equation on the interval $(0, \infty)$

$$-\frac{1}{2}\psi(x) + x\psi(x) = E\psi(x) \tag{3}$$

This ODE was discretized in the following manner:

$$u_{i+1} = u_i - 2(E\psi - x\psi) \tag{4}$$

$$\psi_{i+1} = \psi_i + udx \tag{5}$$

where $u = \psi'$

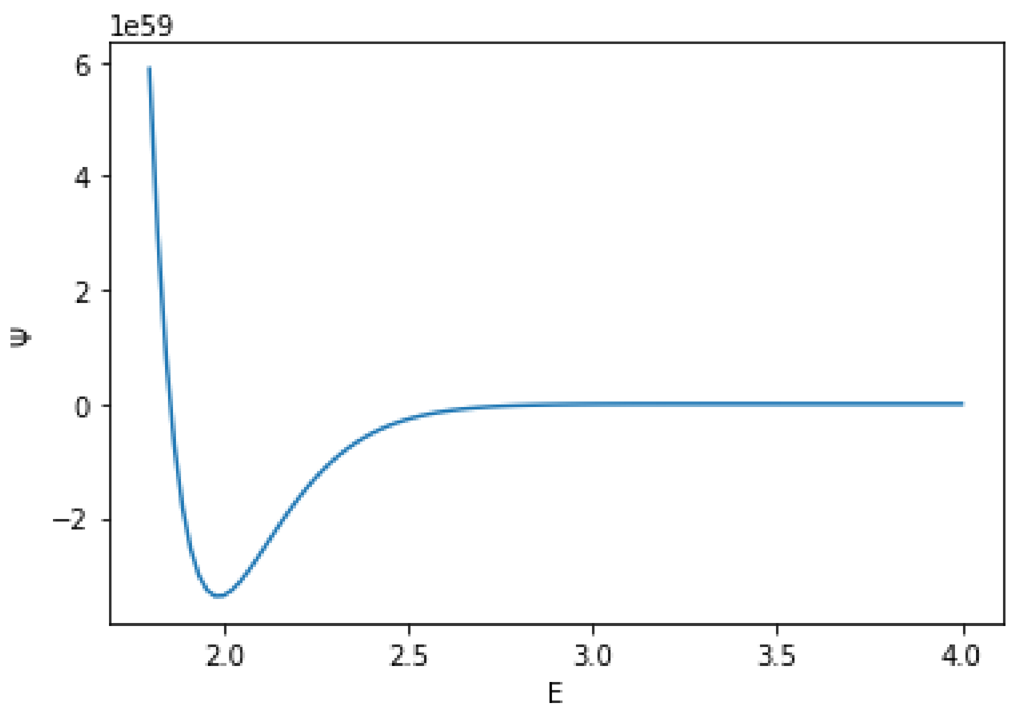
Given an energy, E, and a maximum length, l, the solver first determines the wavefunction on the interval $(0, l)$. Starting with the initial conditions $(x, \psi, \psi') = (0, 0, 1)$, the solver iterates based on the above discretized form of the Schrödinger equation. This continues until a value of $x = l$ is reached, at which point the final value of the wavefunction, $\psi(l)$ is recorded.

This process is repeated over intervals of E and l, resulting in a series of functions of $\psi(l, E)$ where l is the maximum length of integration, and ψ is the final value of the wavefunction recorded at this length. The roots of this function at any given l represent the series of energy eigenvalues of the potential function

$$V(x) = \begin{cases} \infty & x \leq 0, \\ x & 0 < x < l, \\ \infty & x \geq l \end{cases} \tag{6}$$

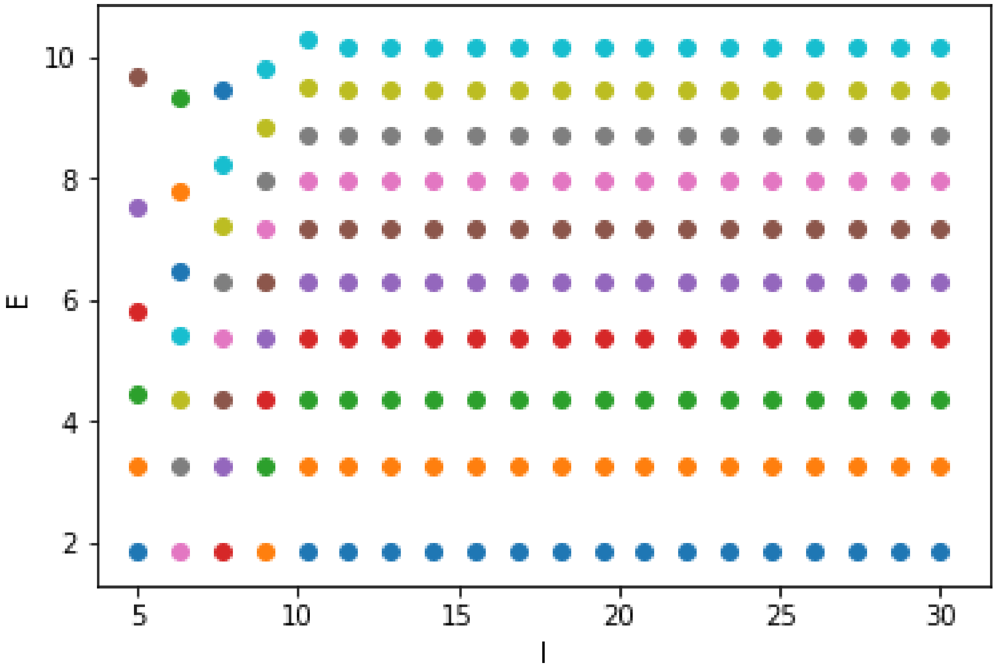
Thus, $\lim_{l\to\infty} \psi(l, E)$ has roots corresponding to the energy eigenvalues of the original potential function (2).

The two root-finding methods we use are Newton's and Bisect. Below, is a figure that shows a ψ at a specific l with varying E values.



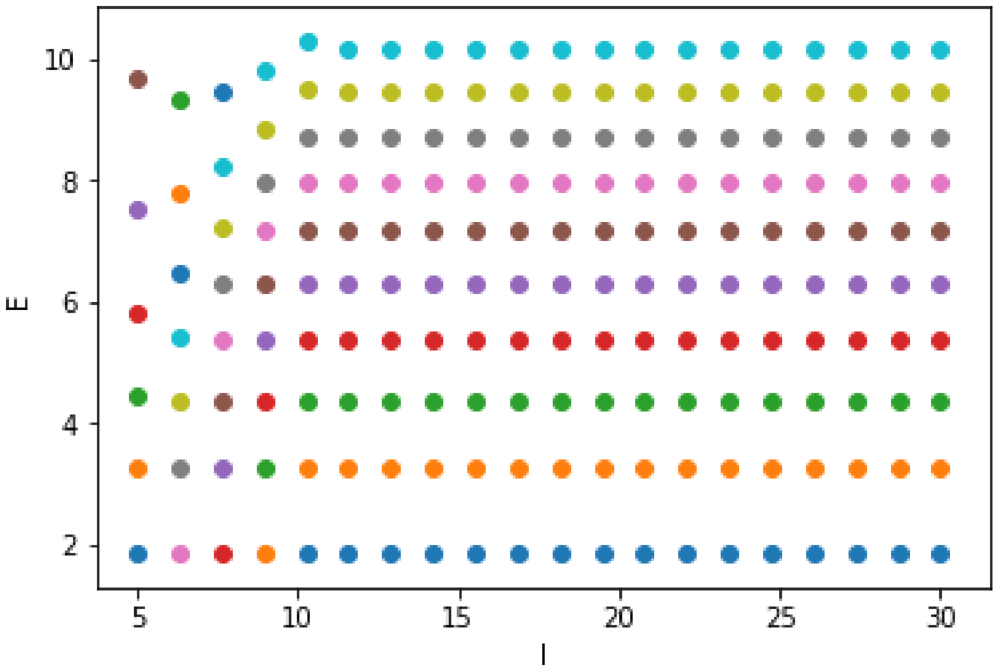
The root-finder determines a series of eigenvalues for which $\psi(l) = 0$. When iterated over a series of values of l, the eigenvaleus converge.

For Newtown's method:



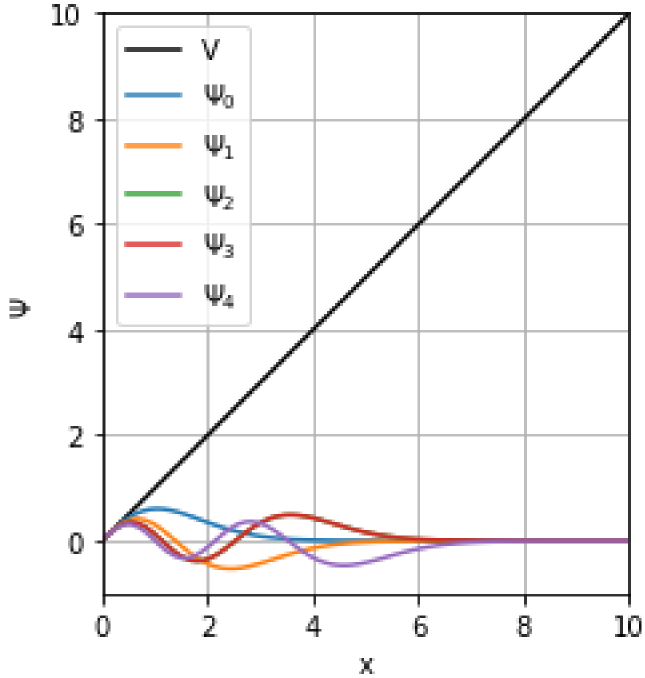
As clearly shown, as l approaches zero, the eigenvalues diverge, and as l increases, the eigenvalues neatly converge.

For the Bisect method:



Extremely similar to Newton's method's results, but the run time was significantly longer.

Corresponding to these eigenvalues, we can determine a series of valid wavefunctions using our discretized equations, (4) and (5).



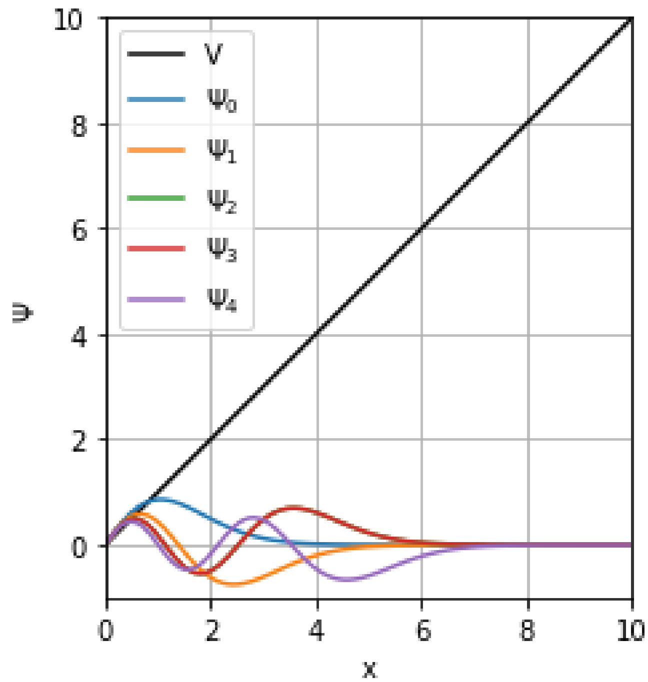
These functions can be modified to satisfy the normalization equation,

$$\int_{-\infty}^{\infty} |\psi|^2 dx = 1 \tag{7}$$

so that the probability of observing the particle on the interval $(-\infty, \infty)$ is 1. By finding this integral for our current wavefunctions, we can find a scalar c such that

$$c \int_{-\infty}^{\infty} |\psi|^2 dx = 1 \tag{8}$$

holds for each function, and scale them accordingly. This yields the following normalized wavefunctions:



Using Mathematica, we came to the following analytical solutiion for $\psi(x)$:

$$\psi(x) = AiryAi[2^{1/3}(x - E)]C_1 + AiryBi[2^{1/3}(x - E)]C_2 \tag{9}$$

This Airy equation nonsense is new to us since we've never taken quantum theory before. However, we understand that it is utilized to solve Schrödinger's equation thanks to Wikipedia.