Chem 302 Laboratory 2

Numerically Solving The Schrödinger Equation for Particle In A Box

NAME:

The Schrödinger equation for a particle in a box is:

\[
-\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} = E \psi
\]

Identify the kinetic energy and potential energy operators.

Using the `Numerov.functions.R` and `Numerov_control.R` scripts, initialize the correct potential and solve this differential equation for a box of length 1.5 length units. Do this for the ground, first and fourth excited states. Print out graphs of the wave functions you obtain.

Describe an algorithm that you could use to normalize the solutions you obtained above. Write out a reasonable pseudo-code.

What is the analytical result for the normalization constant? Show the equation you used to obtain the result. What variables does it depend on?

Use `Numerov.functions.R` and `Numerov_control.R` functionality to numerically normalize the wave functions you obtained. Write down the values computed. Do they agree with the analytical result?

Using the normalization constant(s) you obtained, normalize the un-normalized numerical wave functions you computed with the Numerov procedure. Compute and plot the corresponding normalized probability density curves, connecting the points with
lines. Indicate on the plots where the particle is most likely and least likely to be found. 

*(DO NOT SUBSTITUTE THE PLOT FROM* the `approx.normalize` function! Make your own using the normalization constant produced from `approx.normalize`)*