EXTRA PROBLEM FOR THE MID-TERM P502

Explore the Variational method using the particle in a box (PIB) system by writing a code in python, Matlab or Mathematica.

In order to focus on the variational method, rather than units, we will work in reduced units where most physical constants are equal to 1.

First we define the exact solution to PIB.

$$\psi_k(x) = \sqrt{2}\sin(k\pi x)$$
$$E_k = \frac{k^2\pi^2}{2}$$

a. Plot the first 3 exact solution functions.

b. Calculate the energy eleven for the exact

c. In order to test the variational principle, we need to create a test function that obeys the boundary conditions of the system. We will initially work with

$$\psi(x) = Mx(L - x)$$

where M is a normalization constant. Prove that energy given by

$$E = \frac{\int \psi^* \widehat{H} \psi d\tau}{\int \psi^* \psi d\tau}$$

is greater than the exact ground state energy.
For this purpose:

d. First, make a plot that compares the test function to the exact function. (Note, you will need to normalize the test function to compare it.) Comment on your findings.

e. Normalize your trial function. Plot the the normalized trial functions.

f. Now find the energy of the test function and compare it to the exact value. Does it obey the variational principle?

g. Now let's consider the variational aspect. Namely, let's define a test function that has a parameter that can be varied and see if we can get a better energy. For our test function, we will use

$$f(x) = x(L-x) + Cx^2(L-x)^2$$

where C is an adjustable parameter.

Obtain an expression for the energy of the test function in terms of the parameter C.

h. minimize the energy, i.e. set and find C (Test both roots!)

$$\frac{dE(C)}{dC} = 0$$

K. Compare the exact solution with the one found via the variational principle. Plot both solutions.

l. Compare their energies. Comment how far they are apart.

Attach your code and send as a pdf to your grader for extra points.