AMATH 481/581 - Autumn 2022

Homework #2

Submissions accepted until 11:59 PM (PT) Wednesday, November 2, 2022

To submit this assignment, upload your main homework file (.m, .py, or .ipynb) to Gradescope. Additionally you may upload a .pdf you create to demonstrate mastery of one or both presentation skills.

1. The evolution of the probability function in a one-dimensional harmonic trapping potential is governed by the partial differential equation

$$i\hbar\psi_t + \frac{\hbar^2}{2m}\psi_{xx} - V(x)\psi = 0, \tag{1}$$

where ψ is the probability density, m is the mass, $\hbar$ is Planck's constant, and $V(x) = \frac{kx^2}{2}$ is the harmonic confining potential. A typical solution technique for this problem is to assume a solution of the form

$$\psi(x,t) = \sum_{n=1}^{N} a_n\phi_n(x)\exp\left(-i\frac{E_n}{2\hbar}t\right). \tag{2}$$

This technique is called an *eigenfunction expansion solution* where ϕ_n is an eigenfunction and $E_n > 0$ is the corresponding eigenvalue. Plugging this ansatz into (1) gives the boundary value problem

$$\frac{d^2\phi_n}{dx^2} - [Kx^2 - \epsilon_n]\phi_n = 0, \tag{3}$$

where we expect the solution $\phi_n(x) \to 0$ as $x \to \pm\infty$ and $\epsilon_n > 0$ is the quantum energy. Note that $K = \frac{km}{\hbar^2}$ and $\epsilon_n = \frac{E_n m}{\hbar^2}$. In what follows, take $K = 1$ and always normalize so that $\int_{-\infty}^{\infty}|\phi_n|^2 dx = 1$.

Use the shooting method, as was done in class including using RK45, to calculate the first **five normalized** eigenfunctions (ϕ_n) and eigenvalues (ϵ_n) (up to a tolerance of 10^{-6}) in increasing order such that the **first eigenvalue, $\mathbf{E_1}$, is the smallest one**. For this calculation, use $x \in [-L, L]$ with $L = 4$ and choose `xspan` to consist of $20L + 1$ linearly spaced points between, and including, $-L$ and L. Save the **absolute value** of the eigenfunctions in column vectors (vector 1 is ϕ_1, vector 2 is ϕ_2 and so on) and the eigenvalues in a separate 1×5 **vector**.

Hint 1: Derive the boundary conditions at $\pm L$ as if these are the infinite boundaries, i.e. replacing $x = \pm\infty$ with $x = \pm L$ and performing the derivation that we did in class. Start with an initial guess for the solution at $x = -L$ as $\phi_n(-L) = 1$.

Hint 2: You can check your work as follows. The first eigenfunction, ϕ_1, should have **no** zeros on the interval $[-L, L]$. The eigenfunction ϕ_2 should have **one** zero on $[-L, L]$, etc. Plot your eigenfunctions to see if that is what you are getting.

Deliverables: Save the absolute value of the first 5 eigenfunctions as column vectors to the variables `A1` through `A5`. Save the first 5 eigenvalues in a row vector to the variable `A6`.

For presentation mastery: To demonstrate mastery of creating 3D plots, create a plot of the time evolution of the **second** mode. In other words, create a plot of the function

$$\psi_2(x,t) = \mathrm{Re}\left[\phi_2(x)\exp\left(-i\frac{E_2}{2\hbar}t\right)\right] = \phi_2(x)\cos\left(\frac{E_2}{2\hbar}t\right),$$

versus x and t. Use $x \in [-L, L]$, $t \in [0, 5]$, and $\hbar = m = 1$.

2. We would like to compare the solution found using the shooting method to that using the direct method. To do this, calculate the first **five normalized** eigenfunctions (ϕ_n) and eigenvalues (ϵ_n) in increasing order such that the **first eigenvalue is the lowest one** using the **direct method**. Use all of the same parameters as in Problem 1 (same boundary conditions, $L = 4$, $K = 1$, etc.). Save the **absolute value** of the eigenfunctions in column vectors (vector 1 is ϕ_1, vector 2 is ϕ_2 and so on) and the eigenvalues in a separate 1×5 **vector**.

Hint 1: Formulate the harmonic oscillator as a differential eigenvalue. value problem, i.e.,

$$\left[-\frac{d^2}{dx^2} + Kx^2\right]\phi_n = \epsilon_n\phi_n \tag{4}$$

and discretize it using 2nd order central difference for interior points (without first and last points) to create an eigenvalue problem $A\vec{\phi_n} = \epsilon_n\vec{\phi_n}$ where $\vec{\phi_n} = [\phi_n(x_1), ..., \phi_n(x_{N-1})]$ (assuming that $\vec{x} = [x_0, x_1, \ldots, x_N]$). Such problems can be solved in MATLAB using the `eig` command and in python using `numpy.linalg.eig`.

<u>Hint 2:</u> Use a **bootstrap** approach to determine the boundary equations: To construct the matrix A use the derived boundary conditions (from question 1) and approximate the first and last points using 2nd order forward or backward difference (as appropriate) and assume that Δx is small such that $\Delta x\sqrt{KL^2 - \epsilon_n} \approx 0$. After you found the values of ϕ_n in the interior do not forget to compute the first and last points ($\phi_n(x_0)$ and $\phi_n(x_N)$) using full forward and or backward-difference approximation (without assuming $\Delta x\sqrt{KL^2 - \epsilon_n} \approx 0$). Be sure to save the eigenvectors including the first and last points, i.e., $\vec{\phi_n} = [\phi_n(x_0), \phi_n(x_2), ..., \phi_n(x_N - 1)\phi_n(x_N)]$.

Deliverables: Save the absolute value of the first 5 eigenfunctions as a column vector to the variables `A7-A11`. Save the 5 corresponding eigenvalues in a row vector to the variable `A12`.

3. We would like to explore how nonlinearity plays a role in this problem. To do so, consider

$$\frac{d^2\phi_n}{dx^2} - [\gamma|\phi_n|^2 + Kx^2 - \epsilon_n]\phi_n = 0, \tag{5}$$

with the same boundary conditions and choices of the parameters ($K = 1$) as in the previous problems. You can use the same derived boundary condition as in the previous problems as well. Depending on the sign of γ, the probability density is called *focusing* or *defocusing*. Use the shooting method to find the first two normalized modes (up to a tolerance of 10^{-5}) for $\gamma = 0.05$ and $\gamma = -0.05$. For this calculation, use $x \in [-L, L]$ with $L = 3$ and choose `xspan` to be the vector with $20L + 1$ linearly spaced points between, and including, $-L$ and L. Since this problem is nonlinear, we cannot normalize the eigenfunctions *after* finding a solution to the BVP. Instead, we need to normalize the eigenfunctions and adjust the choice of $\phi_n(-L)$ *in the shooting procedure.* The shooting method changes from only shooting to match the boundary condition to also shooting to match the norm requirement, $\|\phi_n\| = 1$. Please see Homework 2 help pages on Canvas for more information and pseudocode. In the end, save the **absolute value** of the eigenfunctions in column vectors (vector 1 is ϕ_1, vector 2 is ϕ_2) and the eigenvalues in a separate 1×2 **vector**.

Deliverables: For $\gamma = 0.05$, save the absolute value of the two eigenfunctions to `A13` and `A14`, and save the eigenvalues to `A15`. For $\gamma = -0.05$, save the absolute value of the two eigenfunctions to `A16` and `A17`, and the eigenvalues to `A18`.

For presentation mastery: To demonstrate mastery of discussing problems from a mathematical perspective, compare the eigenvalues obtained for the nonlinear model versus those obtained for the linear model. What is the effect of the non-linearity? Do the focusing and defocusing models give different results, if so, how? Do the results surprise you or are they expected? If it helps your discussion to find the eigenvalues with different choices of γ, you may do that.