AMATH 481 & 581 Fall 2018

Homework 2 - Quantum Harmonic Oscillator/Boundary Value Problems

Submission open until 11:59:59pm Thursday October 25, 2018

The probability density evolution 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 and $V(x) = kx^2/2$ is the harmonic confining potential. A typical solution technique for this problem is to assume a solution of the form

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

and is called an eigenfunction expansion solution (ϕ_n=eigenfunction, $E_n > 0$=eigenvalue). Plugging-in this ansatz into Eq. (1) gives the boundary value problem

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

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

Calculate the first **five normalized** eigenfunctions (ϕ_n) and eigenvalues (ε_n) (up to tolerance of 10^{-4}) in increasing order such that the **first eigenvalue is the lowest one** using a shooting scheme. For this calculation, use $x \in [-L, L]$ with $L = 4$ and choose $xspan = -L : 0.1 : L$. 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 **5x1 vector**.

Hint: 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 initial guess for the solution at $x = -L$ as $y(-L) = 1$.

ANSWERS: Should be written out as A1.dat–A5.dat for the eigenfunctions and A6.dat for the eigenvalues.

(2) 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**. For this calculation, use $x \in [-L, L]$ with $L = 4$ and choose $xspan = -L : 0.1 : L$. 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 **5x1 vector**.

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

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

and discretize it using 2nd order central difference for interior points (without first and last points) to receive an e. value problem $A\vec{\phi_n} = \varepsilon_n\vec{\phi_n}$ where $\vec{\phi_n} = [\phi_n(x_2), ..., \phi(x_{N-1})]$. Such problems can be solved in MATLAB using the `eig` command.

Hint 2: 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 and assume that Δx is small such that $\Delta x\sqrt{KL^2 - \varepsilon_n} \approx 0$. After you found the values of ϕ_n in the interior do not forget to compute the first and last points ($\phi_n(x_1)$ and $\phi_n(x_N)$) using full forward or backward-difference approximation (without assuming $\Delta x\sqrt{KL^2 - \varepsilon_n} \approx 0$). Be sure to save the eigenvectors including the first and last points, i.e., $\vec{\phi_n} = [\phi_n(x_1)\ \phi_n(x_2)\ , ...,\ \phi(x_{N-1})\ \phi_n(x_N)]$.

ANSWERS: Should be written out as A7.dat–A11.dat for the eigenfunctions and A12.dat for the eigenvalues.

(3) There has been suggestions that in some cases, nonlinearity plays a role such that

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

Depending upon the sign of γ, the probability density is focused or defocused. Find the first two normalized modes for $\gamma = \pm 0.05$ using shooting. For this calculation, use $x \in [-L, L]$ with $L = 2$ and choose $xspan = -L : 0.1 : L$. 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 **2x1 vector**.

ANSWERS: For γ = 0.05, should be written out as A13-14.dat (eigenfunctions) and A15.dat (eigenvalues). For γ = -0.05, should be written out as A16-17.dat (eigenfunctions) and A18.dat (eigenvalues).

Notes: Use 10^{-4} for the tolerance in shooting methods .