

Quantum Oscillator HW 2A: Using a direct method to solve the ODE

Computational Goal: Find first 5 eigen values/functions ϵ_n for the second order ODE $\frac{d^2\phi_n}{dx^2} - [Kx^2 - \epsilon_n]\phi_n = 0$ with $K = 1$, using the direct method.

1 The domain and boundary conditions?

We are solving the ODE on the same domain as in Homework 1, with the same boundary conditions as specified in the FAQ for Homework 1. With the grid spacing Δx , the domain the finite domain $[-L, L]$ is now discretized with the $n+2$ points $x_0 = -L, x_1 = -L + \Delta x, x_2 = -L + 2\Delta x, \dots, x_{n-2} = L - 3\Delta x, x_{n-1} = L - 2\Delta x, x_n = L - \Delta x, x_{n+1} = L$. The boundaries are the points $x_0 = -L$ and $x_{n+1} = L$. We want to solve for the function values of $\phi_n(x_n)$ at the interior points $x_1, x_2, \dots, x_{n-2}, x_{n-1}, x_n$.

2 Which scheme should I use to discretize the differential equation?

Please use a second order finite difference method (i.e. derived from Taylor series) to discretize the eigen value problem. Recall that with this scheme, a second order derivative at a point x_i in the grid is approximated by:

$$\frac{d^2 f(x_i)}{dx_i^2} \approx \frac{f(x_{i-1}) - 2 * f(x_i) + f(x_{i+1}))}{\Delta x^2} \quad (1)$$

Write the finite difference second order accurate scheme for the ODE at the interior points. You should now have n equations for the n interior points in the domain. Sometimes visualizing the 1D domain as a line segment with the grid points helps with coming up with the equations.

Applying the boundary conditions at $x_0 = -L$ and $x_{n+1} = L$ is a little tricky. Recall that the second order forward and backward schemes for approximating a first order derivative are:

$$\frac{df(x_i)}{dx_i} = \frac{-3f(x_i) + 4f(x_{i+1}) - f(x_{i+2}))}{2\Delta x} \quad (Forward) \quad (2)$$

$$\frac{df(x_i)}{dx_i} = \frac{3f(x_i) - 4f(x_{i-1}) + f(x_{i-2}))}{2\Delta x} \quad (Backward) \quad (3)$$

Applying the forward and backward schemes at the boundaries will give you 2 more equations. The approximation $3 + 2\Delta x\sqrt{KL^2 - \epsilon} \approx 3$ will simplify these equations.

3 What should the discretized system of difference equations derived from the above discretization schemes look like?

The differential equation we are solving is an eigen value-eigen function problem, so when we approximate it to a discretized domain, we would expect to get an eigen value problem. Lets start with the differential equation:

$$\frac{d^2\phi_n}{dx^2} - [Kx^2 - \varepsilon_n]\phi_n = 0 \quad (4)$$

$$\frac{d^2\phi_n}{dx^2} = [Kx^2 - \varepsilon_n]\phi_n \quad (5)$$

So we have a ϕ_n term on both sides of the equation, on the LHS we have a differential operator acting on ϕ_n , on the RHS I have some term multiplying ϕ_n . Discretizing the problem using second order finite difference method, we should get $A * \phi_n = (\text{some term}) * \phi_n$ where the matrix A is a finite difference operator ($\approx \frac{d^2}{dx^2}$). This is again an eigen value problem. Remember that an eigen value problem has the form: $Ax = \lambda x$ where x is an eigen vector of A and λ is the corresponding eigen value. Hint: You can use the MATLAB command `eigs` to find eigen values of A .

4 Could we go through the boundary conditions in detail?

Yes! We will do it here for the steps for the left boundary conditions $x = -L$, with backward difference formula you can work out the same steps for the right boundary condition $x = L$.

The boundary condition is:

$$x = -L : \frac{d\phi_n}{dx} - \sqrt{Kx^2 - \varepsilon_n}\phi_n = 0.$$

With forward difference formula I have:

$$x = -L : \frac{d\phi_n}{dx} \approx \frac{-3\phi_n(x_0) + 4\phi_n(x_1) - \phi_n(x_2)}{2\Delta x}$$

Substituting, I get:

$$x = -L : \frac{-3\phi_n(x_0) + 4\phi_n(x_1) - \phi_n(x_2)}{2\Delta x} - \sqrt{Kx_0^2 - \varepsilon_n}\phi_n(x_0) = 0$$

Now $x_0 = -L$, so I get:

$$x = -L : \frac{-3\phi_n(x_0) + 4\phi_n(x_1) - \phi_n(x_2)}{2\Delta x} - \sqrt{KL^2 - \varepsilon_n}\phi_n(x_0) = 0$$

Rearranging:

$$x = -L : 2\Delta x\sqrt{KL^2 - \varepsilon_n}\phi_n(x_0) = -3\phi_n(x_0) + 4\phi_n(x_1) - \phi_n(x_2)$$

$$x = -L : (3 + 2\Delta x\sqrt{KL^2 - \varepsilon_n})\phi_n(x_0) = 4\phi_n(x_1) - \phi_n(x_2)$$

Use the approximation $3 + 2\Delta x\sqrt{KL^2 - \varepsilon} \approx 3$, we now would have:

$$\phi_n(x_0) = \frac{4\phi_n(x_1) - \phi_n(x_2)}{3}$$

Follow the same steps to get $\phi_n(x_{n+1})$ in terms of interior points $\phi_n(x_n)$ and $\phi_n(x_{n-1})$.

5 A check on matrix A ?

With the above discretizations and approximations, your matrix A should have a well defined structure:

$$\begin{pmatrix} x_1^2 + \frac{2}{3\Delta x^2} & -\frac{2}{3\Delta x^2} & 0 & \cdots & \cdots & 0 \\ -\frac{1}{\Delta x^2} & x_2^2 + \frac{2}{\Delta x^2} & -\frac{1}{\Delta x^2} & & & \\ 0 & & & & & \\ \vdots & & & & & \\ 0 & \cdots & \cdots & -\frac{1}{\Delta x^2} & x_{n-1}^2 + \frac{2}{\Delta x^2} & -\frac{1}{\Delta x^2} \\ & & & -\frac{2}{3\Delta x^2} & x_n^2 + \frac{2}{3\Delta x^2} & \end{pmatrix} \begin{pmatrix} \phi_n(x_1) \\ \vdots \\ \vdots \\ \vdots \\ \phi_n(x_n) \end{pmatrix} = \begin{pmatrix} \varepsilon_n\phi_n(x_1) \\ \vdots \\ \vdots \\ \vdots \\ \varepsilon_n\phi_n(x_n) \end{pmatrix} \quad (6)$$