Assignment 4

Quantum Harmonic Oscillator

November 5th 2024

Exercise: Solve the time independent Schroedinger equation for the quantum harmonic oscillator

$$H = \frac{\hat{p}^2}{2m} + \frac{m\omega^2\hat{x}^2}{2}$$

~~Scaling of the matrix-matrix multiplication. Consider the code developed in the Exercise 3 from Assignment 1 (matrix-matrix multiplication):~~

(a) Write a program to compute the first E_k eigenvalues and $|\Psi_k\rangle$ eigenfunction.

(b) How would you rate your program in terms of the priorities we introduced in class for good scientific software development (Correctness, Stability, Accurate discretization, Flexibility, Efficiency)?

Setting:

Units: $m = \hbar = 1$

1D: $\hat{p} = -i\hbar\nabla_x$

The initial equation reads:

$$H = \frac{1}{2}(-\nabla_x^2 + \omega^2 x^2)$$

One needs to solve the eigenvalue equation:

$$H|\Psi_k(x_i)\rangle = E_k|\Psi_k(x_i)\rangle$$

$$[\frac{1}{2}(-\nabla_x^2 + \omega^2 x^2)]|\Psi_k(x_i)\rangle = E_k|\Psi_k(x_i)\rangle$$

we need to write it as matrix

Method: FINITE DIFFERENCE METHOD

$$[\frac{1}{2}(-\nabla_x^2+\omega^2x^2)]|\Psi_k(x_i)\rangle = E_k|\Psi_k(x_i)\rangle$$

-find approximate solutions by transforming the differential equation into a matrix equations;

- x-axis discretization: divide the interval [a,b] in N intervals: $\Delta x = \frac{b-a}{N}$

important how you discretize

$$[\frac{1}{2}(-\nabla_x^2+\omega^2x^2)] = \hat{K}+\hat{V}$$

K and V do not commute
that's why is a quantum problem-> K cannot be diagonal

Kinetic: $\frac{-\Psi(x_{i+1})+2\Psi(x_i)-\Psi(x_{i-1})}{2\Delta x^2}+\mathcal{O}(\Delta x^2)$

Potential: $V(x_i)=\frac{\omega^2x_i^2}{2}$

OSS Is a sparse matrix: try to use it to check where you can go and compare performances

evaluating the function in three points

$$\hat{K}=\frac{1}{2\Delta x^2}\begin{pmatrix} 2 & -1 & 0 & \dots & 0 & 0\\ -1 & 2 & -1 & \dots & 0 & 0\\ 0 & -1 & 2 & \dots & 0 & 0\\ \vdots & \vdots & \vdots & \dots & \vdots & \vdots\\ 0 & 0 & 0 & \dots & 2 & -1 \end{pmatrix}$$

TRIDIAGONAL

$$\hat{V}=\frac{\omega^2}{2}\begin{pmatrix} x_1^2 & 0 & 0 & \dots & 0 & 0\\ 0 & x_2^2 & 0 & \dots & 0 & 0\\ 0 & 0 & x_3^2 & \dots & 0 & 0\\ \vdots & \vdots & \vdots & \dots & \vdots & \vdots\\ 0 & 0 & 0 & \dots & 0 & x_N^2 \end{pmatrix}$$

Method: FINITE DIFFERENCE METHOD (higher order)

$$[\frac{1}{2}(-\nabla_x^2+\omega^2x^2)]\,|\Psi_k(x_i)\rangle = E_k\,|\Psi_k(x_i)\rangle$$

-find approximate solutions by transforming the differential equation into a matrix equations;

- x-axis discretization: divide the interval [a,b] in N intervals

$$[\frac{1}{2}(-\nabla_x^2+\omega^2x^2)] = \hat{K}+\hat{V}$$

Kinetic: $$\frac{-\Psi(x_{i+2})+16\Psi(x_{i+1})-30\Psi(x_i)+16\Psi(x_{i-1})-\Psi(x_{i-2})}{12\Delta x^2}+\mathcal{O}(\Delta x^4)$$

Potential: $$V(x_i)=\frac{\omega^2x_i^2}{2}$$

$$\hat{K}=\frac{1}{2\Delta x^2}\begin{pmatrix} 5/2 & -4/3 & 1/12 & \dots & 0 & 0 \\ -4/3 & 5/2 & -4/3 & \dots & 0 & 0 \\ 1/12 & -4/3 & 5/2 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \dots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 5/2 & -4/3 \end{pmatrix}$$

PENTADIAGONAL

$$\hat{V}=\frac{\omega^2}{2}\begin{pmatrix} x_1^2 & 0 & 0 & \dots & 0 & 0 \\ 0 & x_2^2 & 0 & \dots & 0 & 0 \\ 0 & 0 & x_3^2 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \dots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 0 & x_N^2 \end{pmatrix}$$

ONCE YOU KNOW HOW TO WRITE DOWN THE HAMILTONIA MATRIX YOU DO A COMPARISON

Discussion: ANALYTICAL COMPARISON

$$\hat{H}\left|\psi_n\right\rangle = \left(\frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2\right)\left|\psi_n\right\rangle = E_n\left|\psi_n\right\rangle$$

the analytical form is provided by Hermite polynomials

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right)$$

eigenvalues

$$\psi_n(x) = \frac{1}{\sqrt{2^n n!}}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega x^2}{2\hbar}} H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right), \qquad n = 0, 1, 2, \ldots$$

eigenfunctions
of the harmonic oscillator

$$H_n(x) = (-1)^n e^{z^2}\frac{\mathrm{d}^n}{\mathrm{d}z^n}\left(e^{-z^2}\right)$$

Hermite polynomials

Discussion: SELF EVALUATION

Correctness —> comparison with analytical solution

Stability —> is the solution stable on different runs?

Accurate discretization —> what does it happen with smaller discretization step?

Flexibility—> can you easily add new functionalities? i.e. higher order

Efficiency —> runtimes?

Report
- introduction with theory
- go through points of assignment

-decide wheter to put code

4 pages

TRY DIFFERENT DELTAS:
what is a "small enough" choice?

APPROFONDIMENTO:
USA METODO IMAGINARY TIME EVOLUTION (HANDS ON) TO FIND THE FIRST EIGENVALUE