Assignment 4

Quantum Information & Computing

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Theory // Schrödinger equation with FDM

Let us consider the **quantum harmonic oscillator** problem

$$\hat{H} = \frac{1}{2m}\hat{p}^2 + \frac{m}{2}\omega^2\hat{x}^2 \qquad \xrightarrow[m=\hbar=1]{1D} \qquad \hat{H} = \frac{1}{2}\left(-\partial_x^2 + \omega^2 x^2\right)$$

$$\hat{H}|\psi\rangle = E|\psi\rangle$$

Taking inspiration from **finite difference methods**, we can approximate the 2^{nd} derivative of ψ as

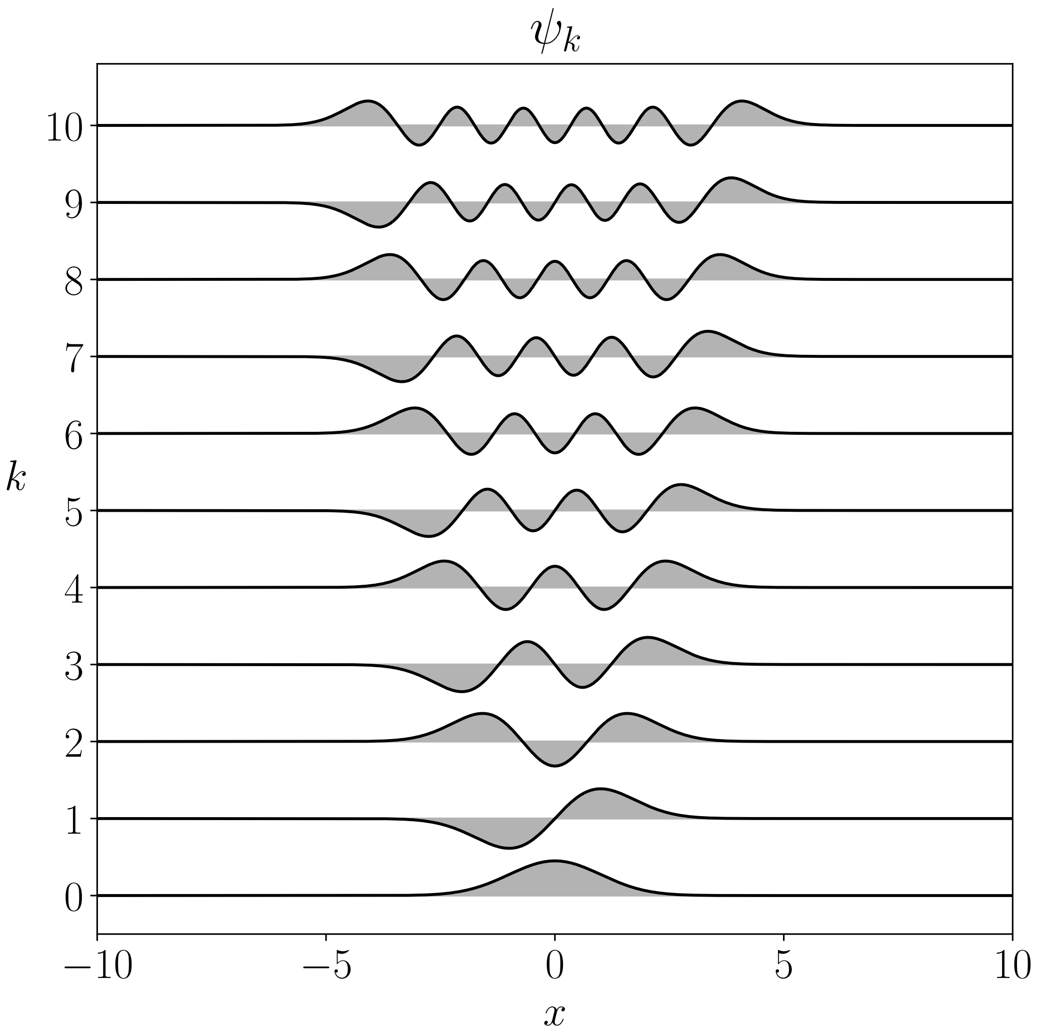
$$\psi''(x_i) = \frac{\psi(x_{i+1}) - 2\psi(x_i) + \psi(x_{i-1})}{dx^2} + \mathcal{O}(dx^2) \qquad \Rightarrow \frac{-\psi(x_{i+1}) + 2\psi(x_i) - \psi(x_{i-1})}{2\,dx^2} + \frac{\omega^2 x_i^2}{2} = E\psi_i$$

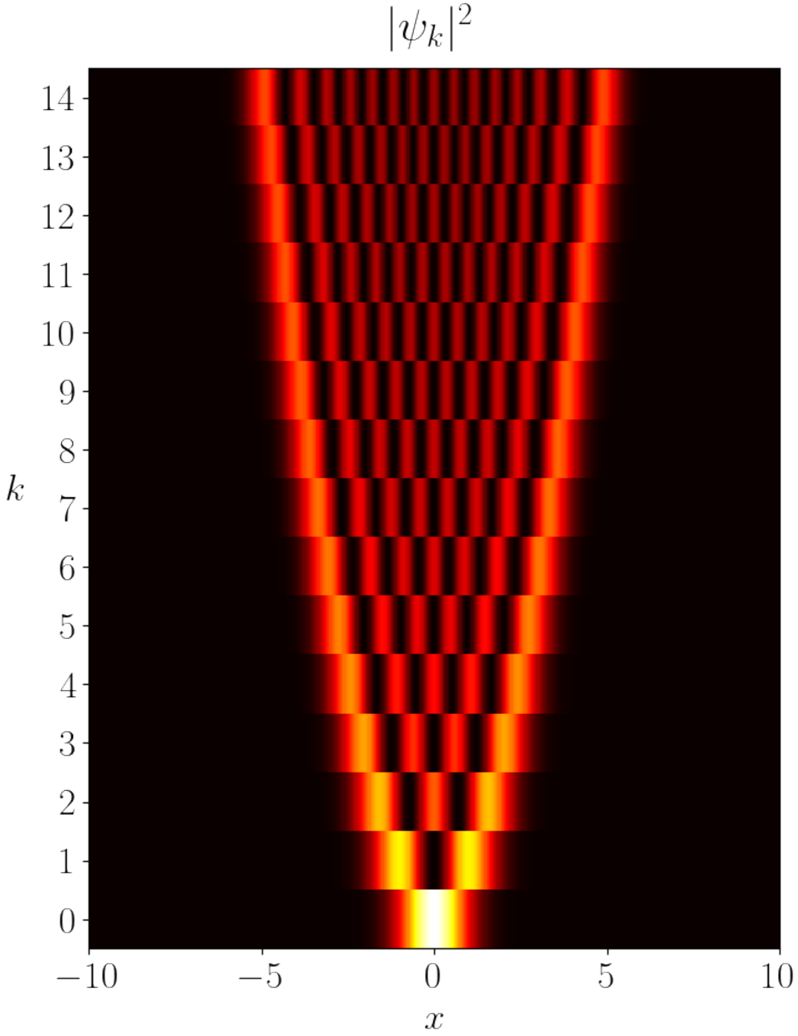
$$\Longrightarrow \hat{H} = \frac{1}{2\,dx^2}\begin{pmatrix} 2 & -1 & & \\ -1 & 2 & & \\ & & \ddots & -1 \\ & & -1 & 2 \end{pmatrix} + \frac{\omega^2}{2}\begin{pmatrix} x_1^2 & & & \\ & x_2^2 & & \\ & & \ddots & \\ & & & x_N^2 \end{pmatrix}$$

i.e. a **tridiagonal eigenproblem**.

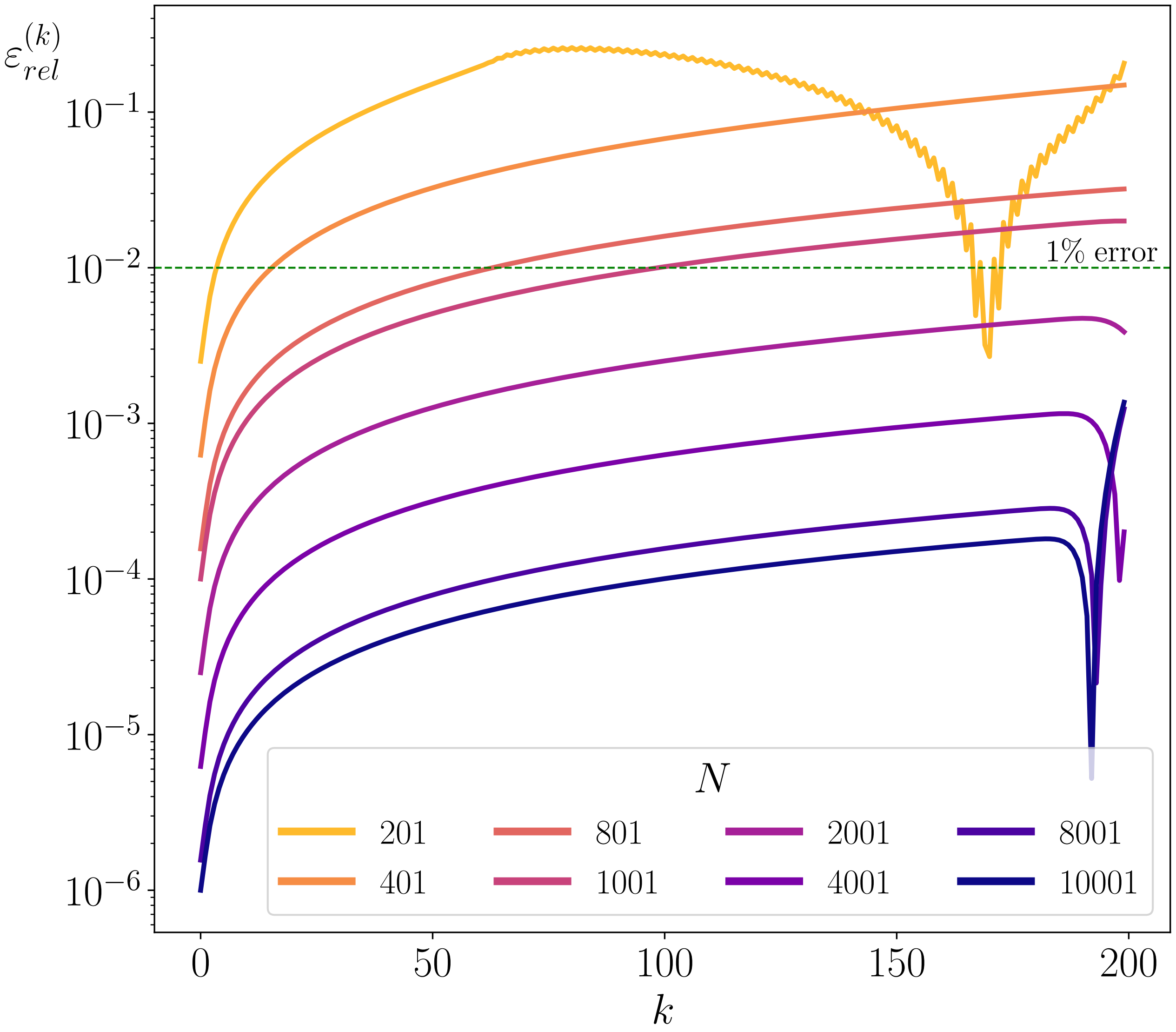
Results // Eigenstates density

The eigenvectors of H are the eigenfunctions ψ_k of the harmonic oscillator ($\omega = 1, m = 1$).
The following plots show an example of **numerical density function** in the interval $x \in [-10.0, 10.0]$.





Results // Eigenvalue relative errors



Let us define the **relative error** on the eigenvalues as

$$\varepsilon_{rel}^{(k)} = \frac{|\varepsilon_{th}^{(k)} - \varepsilon_{num}^{(k)}|}{\varepsilon_{th}^{(k)}}$$

where $\quad \varepsilon_{th}^{(k)} = \omega \left(k + \frac{1}{2}\right)$

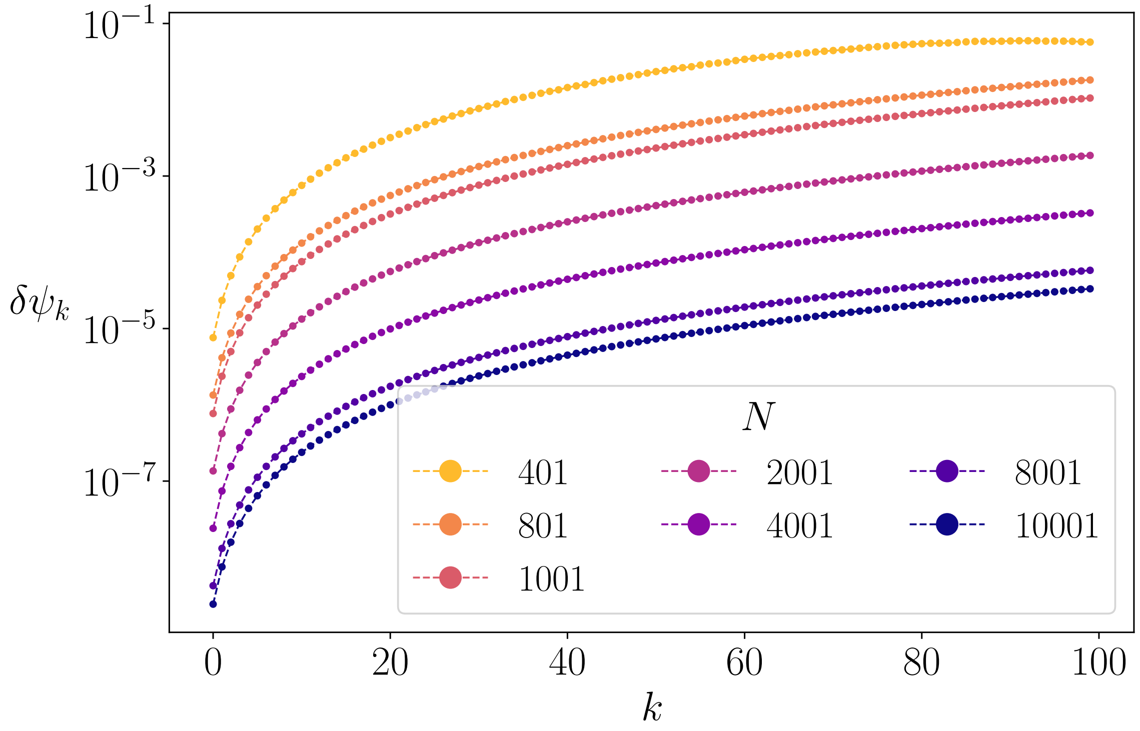
$\varepsilon_{num}^{(k)}$ has been computed using a finite difference method with x discrete variable sampled uniformly N times in the interval $[-20, 20]$.

We see that for all the **first** $k = 200$ **eigenvalues** the relative error is below the threshold of 1% if $N > 2001$.

Results // Eigenfunction errors

To characterize the **error on the eigenstates**, we have considered the norm-1 metric:

$$\delta\psi_k^{(N)} = \frac{1}{N}||\psi_k^{th}(x_i) - \psi_k^{num,N}(x_i)||_1$$



How would I rate my program?

The software is *stable* for large matrix size. A bash script allows us to be *flexible* in the variation of the harmonic oscillator parameters, N in particular.

As of *efficiency*, I used a specific routine (dsbevx) to diagonalize real symmetric band matrices (tridiagonal is a special case).

A side advantage of such choice, is that the hamiltonian is stored already in **upper-band-packed mode** (ref: IBM ESSL), optimizing the memory usage down to $\mathcal{O}(N)$. Eventually, binary files have been used to dump the eigenvectors and do the post processing in Python (as csv files would be too big).

Hopefully, the software is *correct* & the *accuracy* of the discretization has been proved by the previous plots.

Improvements // Higher order finite difference method

Finite difference methods can be taken to **higher orders**... for instance

Can we
do better?

$$\psi''(x_i) = \frac{-\psi(x_{i-2}) + 16\psi(x_{i-1}) - 30\psi(x_i) + 16\psi(x_{i+1}) - \psi(x_{i+2})}{12\ dx^2} + \mathcal{O}(dx^4)$$

$$\implies \quad \hat{H} = \frac{1}{2\ dx^2}\begin{pmatrix} 5/2 & -4/3 & 1/12 & 0 & \dots & 0 \\ -4/3 & 5/2 & -4/3 & 1/12 & & \vdots \\ 1/12 & -4/3 & & & & 0 \\ 0 & & & \ddots & \vdots & 1/12 \\ \vdots & & & \dots & 5/2 & -4/3 \\ 0 & \dots & 0 & 1/12 & -4/3 & 5/2 \end{pmatrix} + \frac{\omega^2}{2}\begin{pmatrix} x_1^2 & & & \\ & x_2^2 & & \\ & & \ddots & \\ & & & x_N^2 \end{pmatrix}$$

Now the approximation is correct up to 4th order in dx, **H is pentadiagonal** but still solvable with DSBEVX.

Improvements // Pentadiagonal FDM

These plots prove that **an higher order finite difference method is very effective**.
Indeed, the accuracy of the first $k = 200$ eigenproblem solutions improves by <u>several orders of magnitude</u>.