EXERCISE 4
CONTINUOUS TIME-INDEPENDENT SCHRODINGER EQUATION

QUANTUM INFORMATION AND COMPUTING COURSE 2021/2022

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EXERCISE GOALS

Consider the one-dimensional quantum harmonic oscillator defined by the Hamiltonian

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

- Write a Fortran program to compute the first k eigenvalues E_k and eigenvectors $|\psi_k\rangle$.
- Rate your program in terms of the priorities for good scientific software development (Correctness, Stability, Accurate discretization, Flexibility, Efficiency)

WHAT SHOULD I EXPECT?

- Theory of quantum mechanics: eigenvalues in the form $E_n = 2\times(n + {}^1/_2)\hbar\omega$ $\Rightarrow$ constant difference among eigenvals
- Eigenfunctions: Hermite functions (# of nodes $= n$)
- Finite size: discretize second derivative operator in $\hat{p}^2$ as

$$\psi_n{}'' = \frac{\psi_{n-1} - 2\psi_n + \psi_{n+1}}{\Delta x^2} + \vartheta(\Delta x^4)$$

- At the boundaries, expected no kinetic contribution: for $x \in [-L, L]$

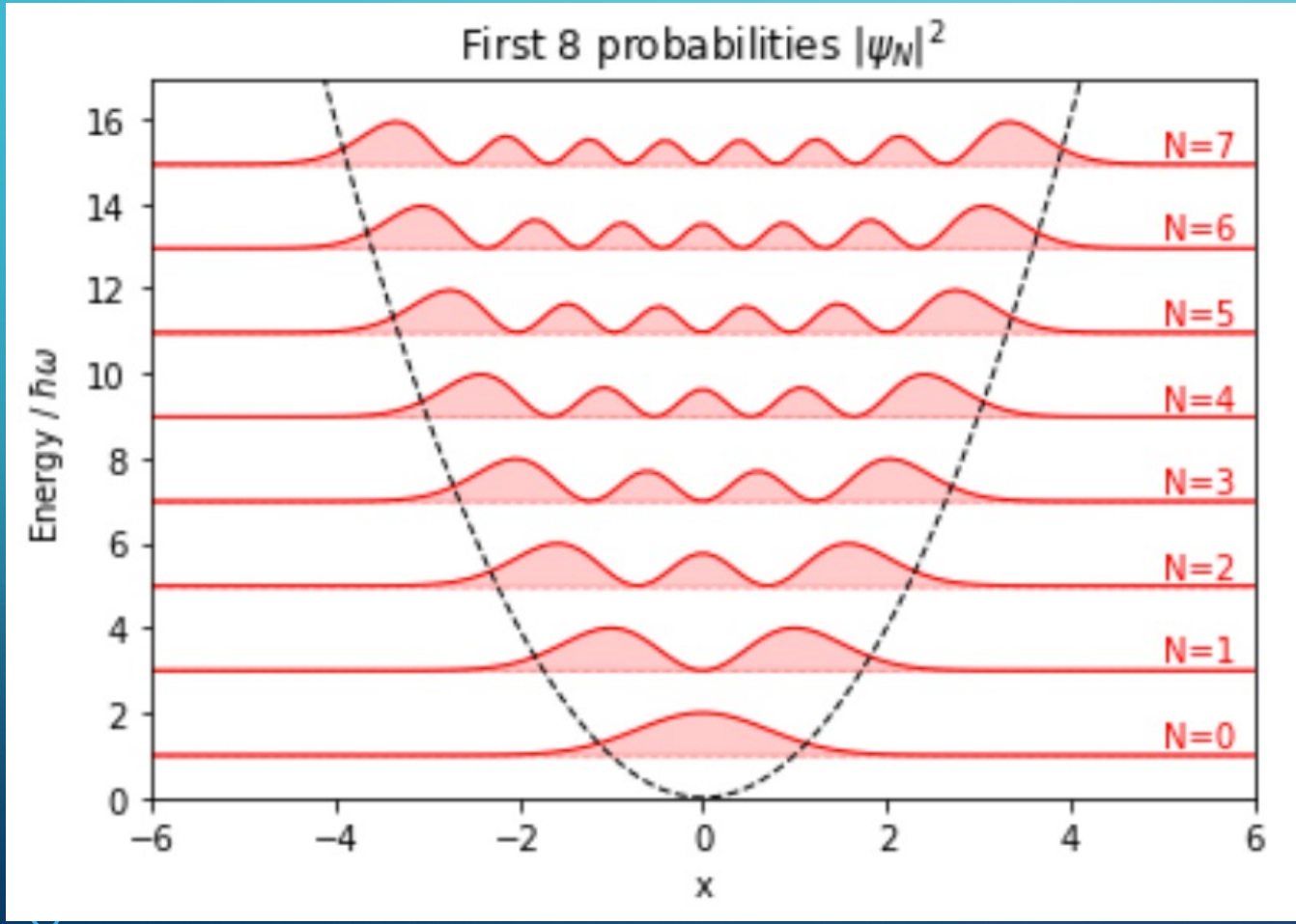
$$\omega^2 L^2 = E_n \Rightarrow L = \sqrt{E_n}/\omega$$

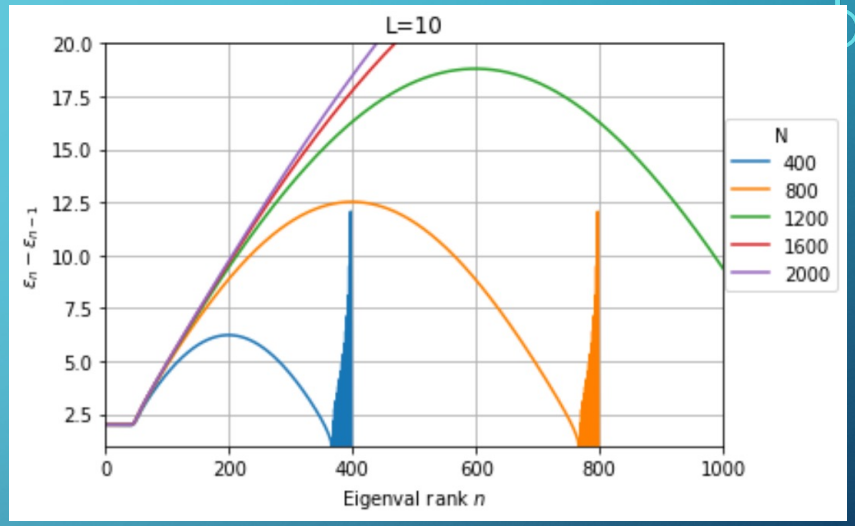
CODE DEVELOPEMENT

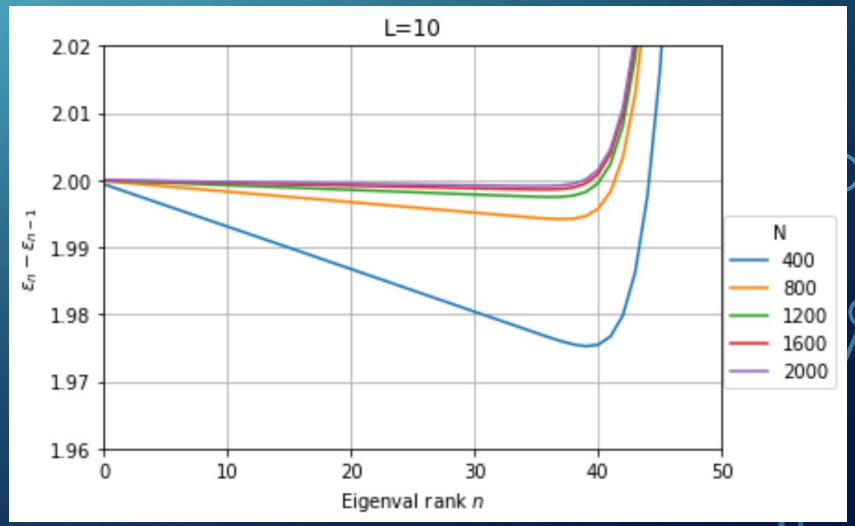
```
V_diag = (X**2)*(omega**2)

D = (2./(dx**2))*hbar**2 + V_diag
E = [(-1.,ii=1,N-1,1)]*(1./(dx**2))*hbar**2

call DSTEV( 'V', N, D, E, Z, LDZ, WORK, INFO )
```

- Use of LAPACK's DSTEV for hamiltonian diagonalization
- Avoid defining zero elements to improve efficiency and reduce memory use
- Add pre-conditions on input variables (e.g, non-negative discretization interval and number of points
- Add post-condition on exit status of DSTEV

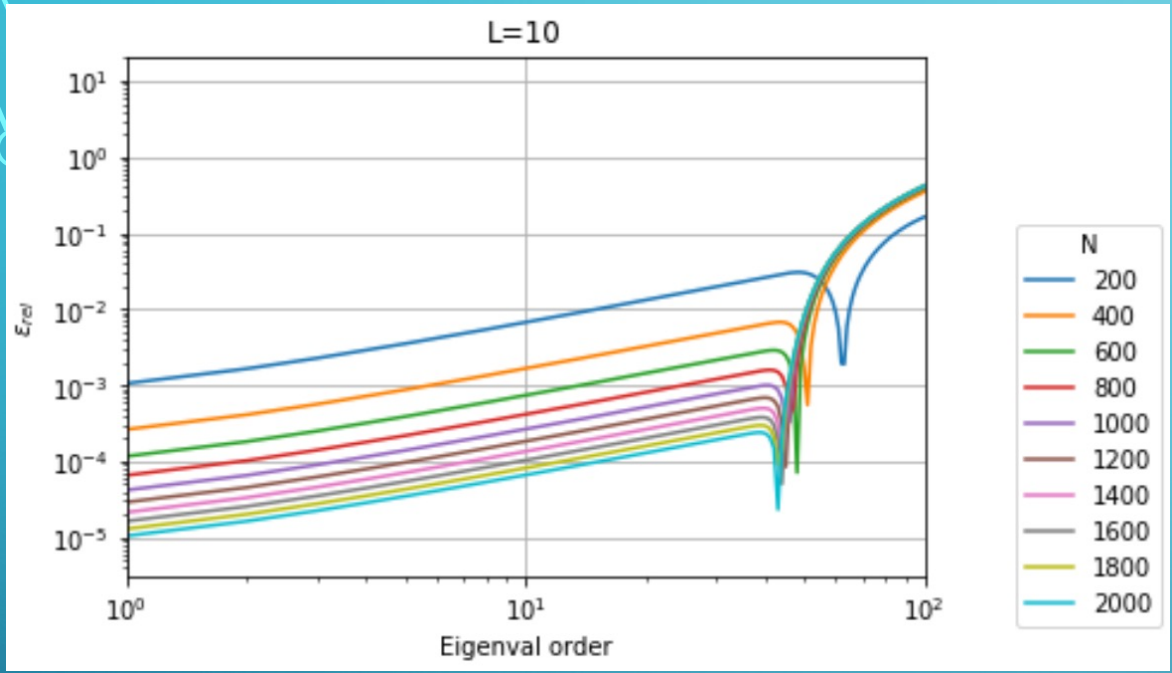
RESULTS – PDFS AND DEPENDENCE ON N

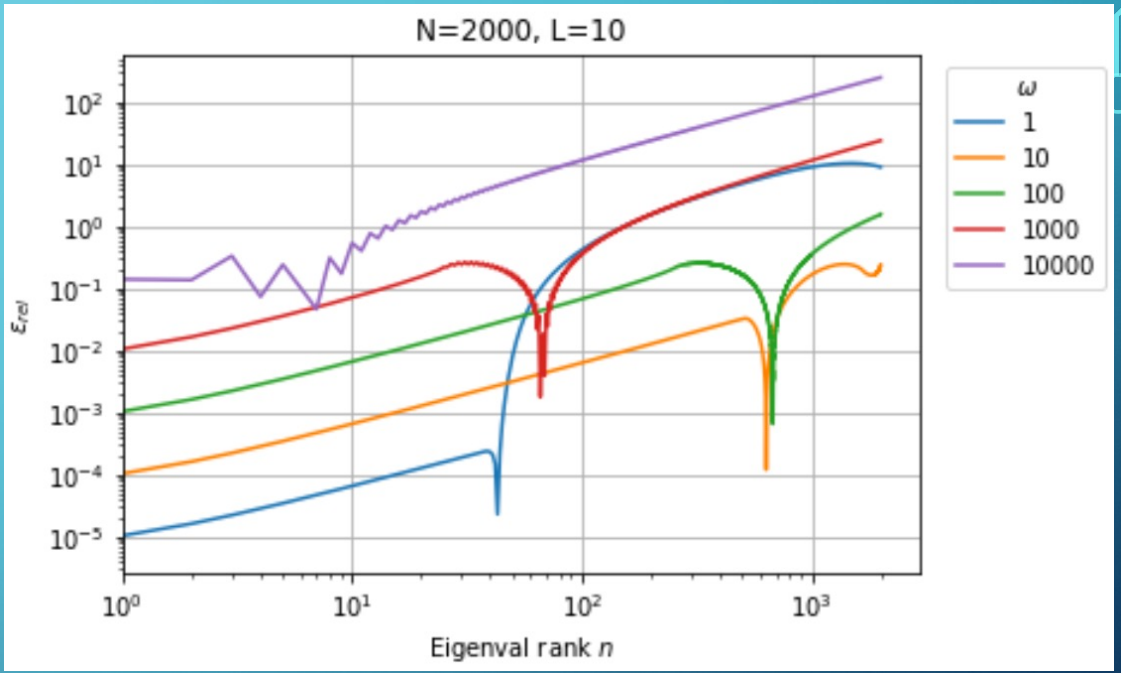






RESULTS – DEPENDENCE ON L AND ω





FINAL OVERVIEW

It is hard to keep under control the whole algorithm: by one side, a larger L allows to estimate better higher level eigenvalues, the quality on the first ones. Similarly, a larger N allows for better precision on first energy levels, by it must be set wrt L. Changing ω means scaling the eigenvals: the last plot suggest that it must also be taken into consideration while setting the best N, L.