Week 4 assignment

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Quantum Information and Computation

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Analytical solution

$$\hat{H} = \frac{1}{2}\hat{p}^2 + \frac{1}{2}\omega^2\hat{q}^2$$

- $\omega = 1$, natural units $\hbar = 1$
- x-position representation: $\hat{p} \to -i\hbar\frac{\partial}{\partial x}$, $\hat{q} \to x$

$$\hat{H}\psi = E\psi \to \left(-\frac{\hbar^2}{2}\frac{\partial^2}{\partial x^2} + \frac{1}{2}x^2\right)\psi_n(x) = E_n\psi_n(x)$$

Theoretical eigenvalues and eigenvectors: $E_n = \left(n + \frac{1}{2}\right)\hbar\omega$

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

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

$$\psi_k'' = \frac{\psi_{k+1} - 2\psi_k + \psi_{k-1}}{(\Delta x)^2} + \mathcal{O}(\Delta x)^4$$

End up with tridiagonal Hamiltonian

$$\begin{bmatrix} \frac{1}{(\Delta x)^2} + \frac{1}{2}\omega^2 x_1^2 & -\frac{1}{2(\Delta x)^2} & 0 & \cdots & 0 \\ -\frac{1}{2(\Delta x)^2} & \frac{2}{2(\Delta x)^2} + \frac{1}{2}\omega^2 x_2^2 & -\frac{1}{2(\Delta x)^2} & \cdots & 0 \\ 0 & -\frac{1}{2(\Delta x)^2} & \ddots & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \cdots & \cdots & \cdots & \cdots & \frac{1}{(\Delta x)^2} + \frac{1}{2}\omega^2 x_N^2 \end{bmatrix}$$

Interval $[-a, a]$, discretization step $\Delta x = \frac{a}{N}$.

Compile: gfortran harmonicL.f90 -o harm -llapack
Input: a, N, ω

```
do ii = 0, 2*N
        grid(ii+1) = -a + ii*dx
end do
```

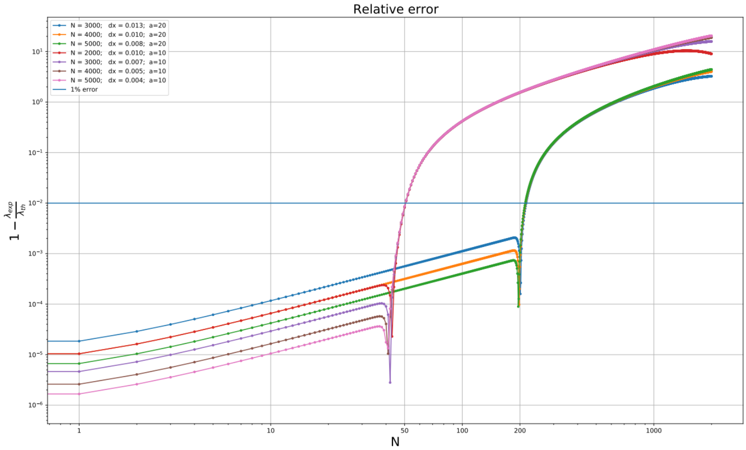
```
do ii = 1, size(grid,1)
                d(ii) = 1d0/(dx**2d0) +  (omega**2d0 * grid(ii)**2d0)/2d0
end do

do ii = 1, size(grid,1)-1
        sub_d(ii) = -1d0/(2d0*dx**2d0)
end do
```

Tridiagonal symmetric matrix; out d = eigenvalues, Z = eigenvectors

```
call DSTEV('V', dimension, d, sub_d, Z, dimension, WORK, INFO)
```

Plot $\epsilon_n = \frac{|\lambda_{th,n} - \lambda_{exp,n}|}{\lambda_{th,n}}$.

$a = 10$ solution reaches 1% error around $N \approx 50$, while $a = 20$ at ≈ 200.



Quadratic behaviour $\rightarrow E_n = \frac{\pi^2}{2L^2} n^2$ for a particle in a box. $V(x)$ is infinite outside $[-a, a]$

- **Correctness** Agreement with theory within 1% error up to ≈ 40 eigenfunctions.
- **Numerical Stability** Code was tested with many inputs and relies on LAPACK.
- **Accurate Discretization** Large enough interval, *dx* should be neither too little or big (bad sampling)
- **Flexibility** a, ω should be integers for scripting convenience. Flexible as long as you stick to tridiagonal symmetric matrices.
- **Efficiency** DSTEV from LAPACK. Could have optimized workspace.