UNIVERSITÀ DEGLI STUDI DI PADOVA

Quantum Information and Computing

2021 - 2022

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Solution of the Time Independent Schrödinger Equation for an harmonic oscillator

Physics of Data

Theory

$$\begin{cases} \hat{H} = \hat{p}^2 + \omega^2 \hat{x}^2 \quad \text{where } \hbar \equiv m \equiv 1 \\ \hat{H}\psi = E\psi \\ \hat{p} \to -i\hbar\partial/\partial x, \quad \hat{x} \to x \end{cases} \Rightarrow \begin{cases} \left(-\frac{1}{2}\frac{\partial^2}{\partial x^2} + \frac{1}{2}\omega^2 x^2\right)\psi(x) = E_n\psi(x) \\ \psi_k'' = \frac{\psi_{k+1} - 2\psi_k + \psi_{k-1}}{dx^2} \end{cases}$$

$$\equiv \quad -\frac{1}{2}\left[\frac{\psi_{k+1} - 2\psi_k + \psi_{k-1}}{dx^2}\right] + \frac{1}{2}\omega^2 x_k \psi_k = E\psi_k$$

$$H = \frac{1}{2}\begin{pmatrix} \frac{2}{dx^2} + \omega^2 x_1^2 & -\frac{1}{dx^2} & 0 & \cdots & 0 \\ -\frac{1}{dx^2} & \frac{2}{dx^2} + \omega^2 x_2^2 & -\frac{1}{dx^2} & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & \frac{2}{dx^2} + \omega^2 x_N^2 \end{pmatrix} \Longleftrightarrow H\psi = E\psi$$

Code Development

qho_H_init() in module qho:

Initialize the complex matrix to represent the hamiltonian of the system given L and N

```
function qho_H_init(L,N,omega) result(H)
  real                                  :: L,omega,dx
  integer                               :: N, ii
  real*16, dimension(:,:), allocatable  :: elem_real
  type(cmatrix)                         :: H
  dx = L/N

  allocate(elem_real(N+1,N+1))
  elem_real = 0 * elem_real ! Initialize everything to 0

  do ii=1, N+1, 1 ! ! diagonal elements
    elem_real(ii,ii) = ( 2 /(dx**2) ) + (omega**2)*((ii-1)*dx - L/2)**2
  end do

  do ii=2, N+1, 1 ! tridiagonal elements
    elem_real(ii,ii-1) = - 1/(dx**2)
    elem_real(ii-1,ii) = - 1/(dx**2)
  end do

  elem_real = 0.5* elem_real ! Everything must be divided by 2

  H = cmatrix_init(cmplx(X=elem_real,KIND=8))
end function qho_H_init
```

ZGEEV() function in LLAPACK library:

For eigenvalues and eigenvectors

```
call ZGEEV(! To compute both eigenvalues and -vectors
           'V', 'V', &
           ! The order of the matrix A
           N, &
           ! The matrix
           A, &
           ! The leading dimension of A.
           N, &
           ! Where to store eigenvalues and eigenvectors
           eigenv, eigenh, &
           ! Other parameters
           N, VR, N, WORK,LWORK,RWORK, &
           ! Output parameter, if INFO == 0 -> successful exit
           INFO      )
```

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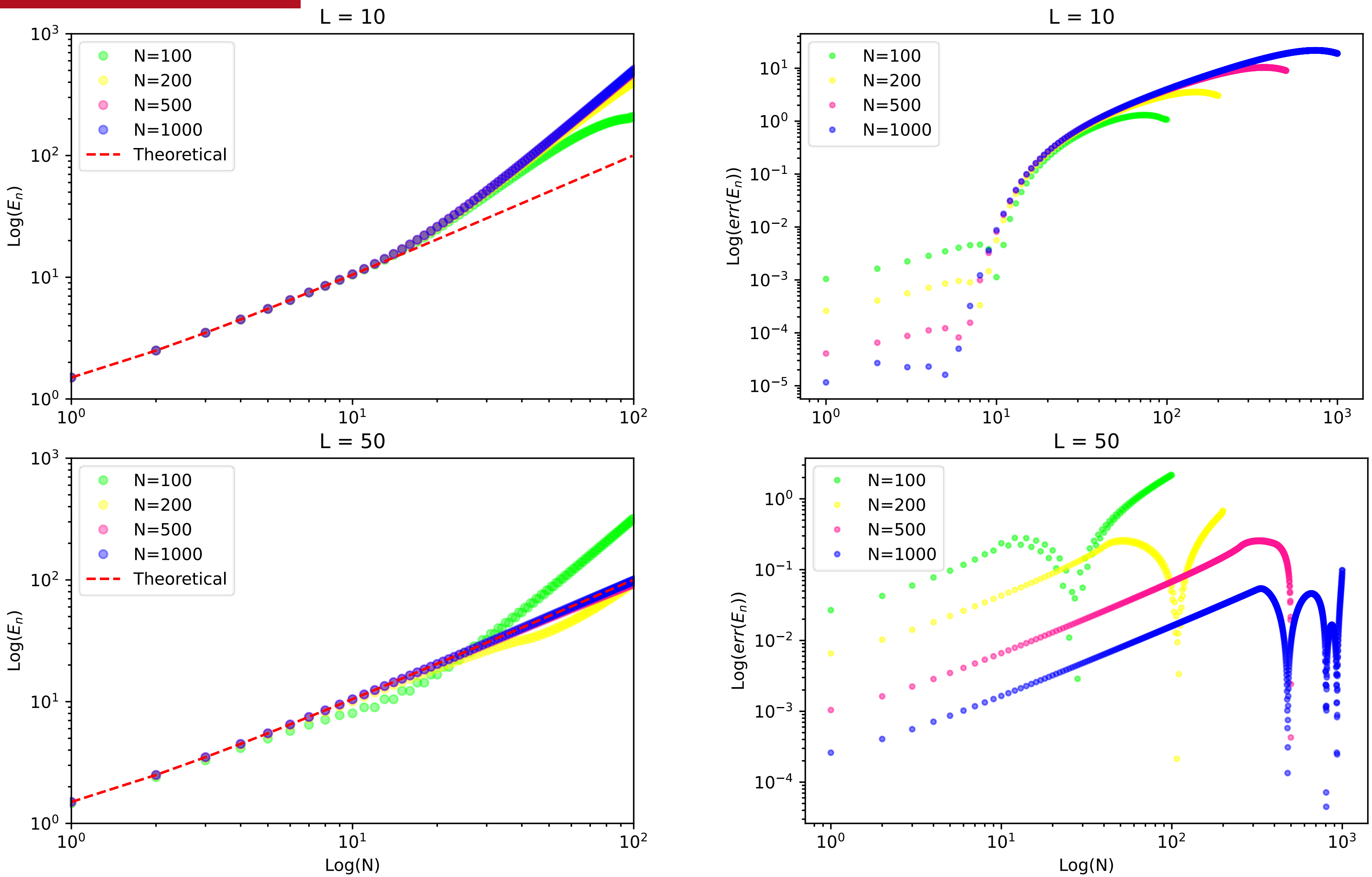
Results

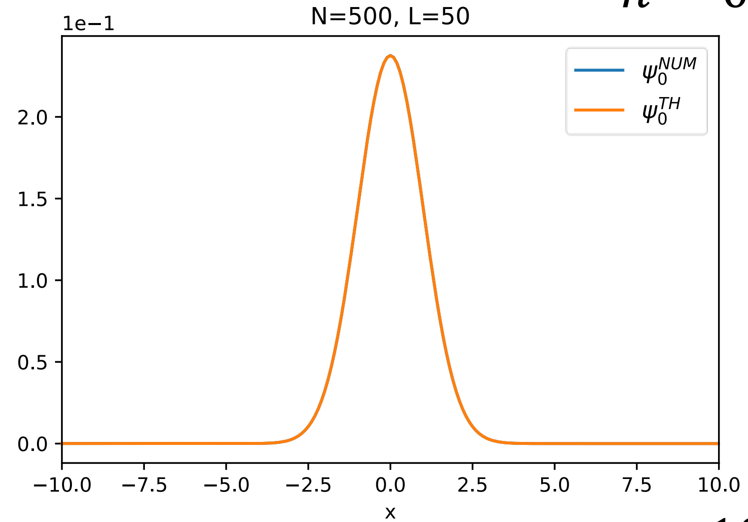
$$err(E_n) \equiv \frac{|E_n - E_n^{true}|}{E_n^{true}}$$

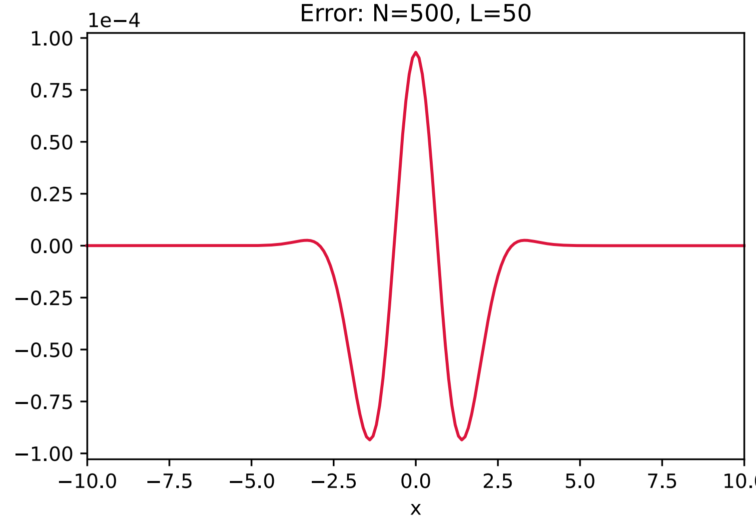


Results

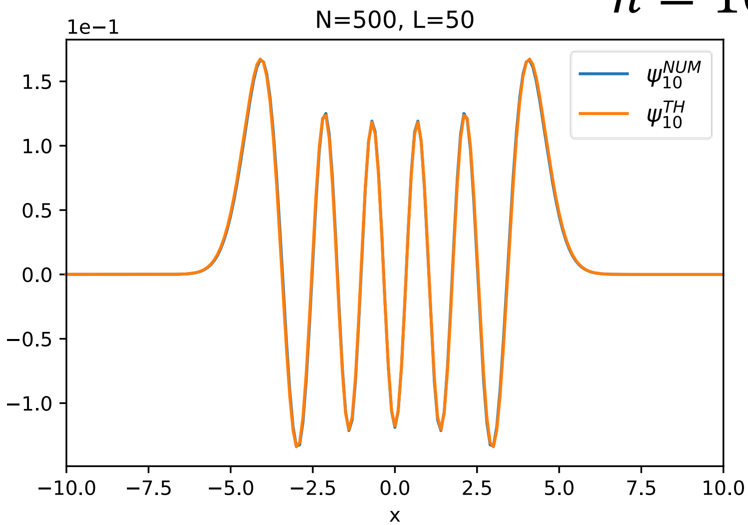
$$err \equiv \psi_i^{num} - \psi_i^{th}$$

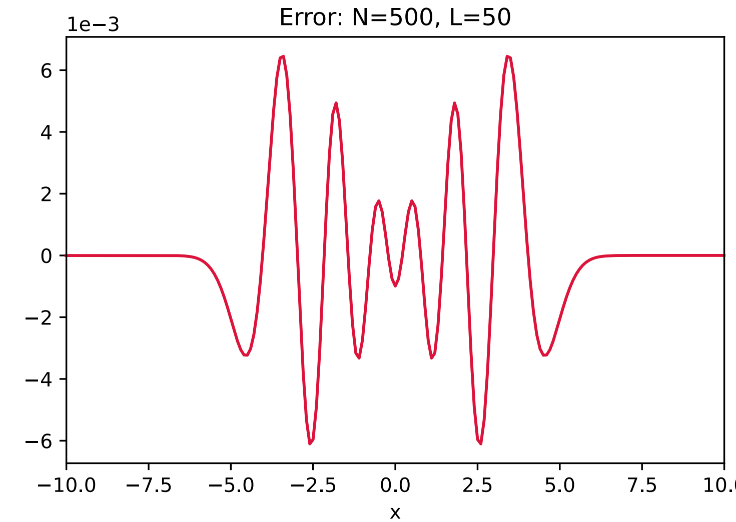
$n = 0$





$n = 10$





Self evaluation

Correctness: Hugely depends on the choice of the parameters. It can be still improved by using a better formula for the derivative

Stability: Various checks have been implemented to make the program as stable as possible

Accurate discretization: For the right parameters (for example L=50 and N=1000) the programs gives accurate results

Flexibility: Based on ZGEEV and not DSTEMR for generalizing to other problems

Efficiency: Can be improved by considering DSTEMR and real-only matrices

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Thanks for the attention