UNIVERSITÀ DEGLI STUDI DI PADOVA

Quantum Information and Computing

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Exercise #03

Physics of Data

Theoretical

We consider the 1D quantum harmonic oscillator:

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

The eigenvector can be found from the above:

$$\longrightarrow \quad -\frac{1}{2}\left[\frac{\psi_{k+1} - 2\psi_k + \psi_{k-1}}{dx^2}\right] + \frac{1}{2}\omega^2 x_k \psi_k = E\psi_k \quad \text{where} \quad H_{ij} = <\psi_i|H|\psi_j>$$

We can get the matrix:

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

Time Independent Schrödinger Equation

Code development

We created the function to initialize the complex matrix to represent the Hamiltioian of the system given by L and N.

We create the subroutine to compute the eigenvalues and eigenvectors.

```
function qho_H_init(L,N,omega) result(H)
  real            :: L,omega
  integer         :: N, ii

  real*16, dimension(:,:), allocatable :: elem_real
  type(cmatrix)                        :: H

  allocate(elem_real(N+1,N+1))
  elem_real = 0 * eleam_real

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

  do ii=2, N+1, 1
    elem_real(ii,ii-1) = - (N*N)/(L*L)
    elem_real(ii-1,ii) = - (N*N)/(L*L)
  end do

  elem_real = 0.5* elem_real

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

```
subroutine cmatrix_herm_eigens(cmat,eigenv,eigenh,success)
  type(cmatrix)                                      :: cmat
  real*8, dimension(:)                               :: eigenv
  complex(kind=8), dimension(:,:)                    :: eigenh
  integer, optional                                  :: success

  ! LAPACK variables
  double precision, dimension(:), allocatable          :: RWORK
  integer                                              :: INFO, LWORK
  integer                                              :: N
  integer, parameter                                   :: LWMAX = 100000
  complex*16                                           :: WORK(LWMAX)
  complex(kind=8), dimension(:,:), allocatable         :: VR
  ! Check if matrix is squared
  if(cmat%dim(1) == cmat%dim(2)) then
    N = cmat%dim(1)

    allocate(RWORK(3*N-2))
    allocate(VR(N,N))

    ! Compute optimal size of workspace
    LWORK = -1
    eigenh = cmat%element

    call ZHEEV('Vectors', 'U', N, eigenh, N, eigenv, WORK,LWORK,RWORK,INFO)
    LWORK = min(LWMAX, int(WORK(1)))

    ! Compute eigenvalues
    call ZHEEV('Vectors', 'U', N, eigenh, N, eigenv, WORK,LWORK,RWORK,INFO)

    if(present(success)) then
      success = INFO
    end if
  end if
end subroutine cmatrix_herm_eigens
```

Results

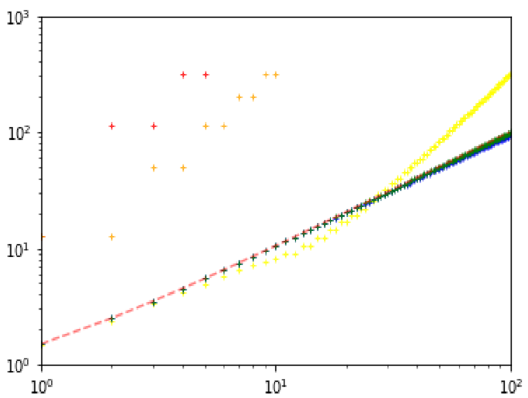
```
qi@qi-VirtualBox:~$ gfortran schro-eq.f90 -o schro-eq eigen -llapack
qi@qi-VirtualBox:~$ ./schro-eq
 +            QUANTUM HARMONIC                     +
 ----------------------------------------------------------
 + Type: L, N, omega and folder name: 1
1000
1
qho
 + Data will be saved in: ./qho
 + Lenght of x space (L):     1.00000000
 + Number of points   (N):          1000
 + Angular frequency (ω):     1.00000000

 + Computing the Hamiltonian...
  !!! H matrix is too big to be printed on screen !!!

 + Computing Eigenvalues & Eigenvectors...
   Eigenvalues:
     4.92671108
     19.6926308
     44.2757454
     78.6756668
     122.907829
   writing on file: ./qho/eigenvalues.csv
   writing on file: ./qho/eigenvectors.csv

 Done!
```

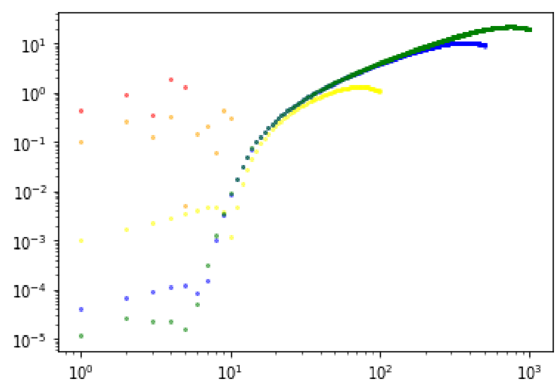
Time Independent Schrödinger Equation

Results

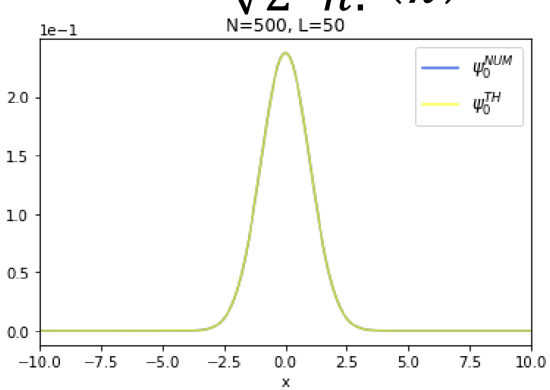
$$E_n^{true} = \omega\left(n + \frac{1}{2}\right)$$

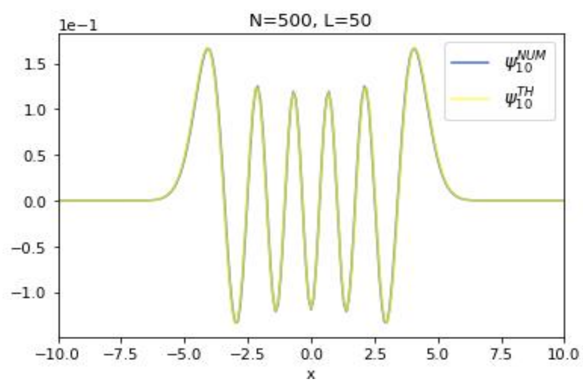
$$err(E_n) \equiv \frac{|E_n - E_n^{true}|}{E_n^{true}}$$





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





Time Independent Schrödinger Equation

Correctness: The code provides results in accordance with theoretical expectation but it highly depends on the choice of the parameters.

Stability: The code has been run multiple times in order to make the program as stable as possible.

Accurate discretization: The discretization can be improved by modifying the input parameters, (for L=50 and N = 1000, it returns the accurate results).

Flexibility: The program can be adapt in different values of parameters.

Efficiency: Can be improved by considering as real-only matrices.

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Thanks for the attention