Continuous time-indipendent Schrödinger Equation

1 Abstract

In this exercise we wrote a program able to compute eigenvalues and eigenfunctions for a time-independent quantum oscillator.
During code execution we implement many checks in order to avoid miscalculations or bad initialization of parameters and in order to evaluate how much time each part takes.

2 Theory

The hamiltonian matrix's system is :

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 \tag{1}$$

In the space representation it becomes:

$$H = -\frac{\hbar^2}{2m}\partial_x^2 + \frac{1}{2}m\omega^2 x^2 \tag{2}$$

This system shows a characteristic parameter called *typical lenght* defined as follows :

$$x_0 = \sqrt{\frac{\hbar}{m\omega}} \tag{3}$$

if we substitute this x_0 into harmonic potential defined as $V_{(x)} = \frac{1}{2}m\omega^2 x^2$ we obtain $\frac{1}{2}\hbar\omega$ that is so called *ground state* .

In order to solve this equation by computer we need to discretize everything and in particular we have that ∂_x^2 becomes :

$$\frac{d^2\psi}{dx^2}(x_k) = \frac{\psi_{k+1} - 2\psi_k + \psi_{k-1}}{\epsilon^2} + \ o(\epsilon^2) \tag{4}$$

where ϵ is the discretized interval width and for potential function we have

$$V(x_i) = \frac{1}{2}m\omega^2 x_i^2 \tag{5}$$

Obviously we need to fix a priori *system length* L and so the interval $[-L, L]$ where particle will be placed . Then this value will be modulated by ϵ in order to achieve as much as possible details and precision about eigenvalues and eigenfunctions.
In synthesis ,given L,the *effective length* will be L'=ϵL.

Fixing ϵ and L we have two limits: the first one is for high energies and its theoretical value is $E_{upper} = \frac{\hbar^2}{2m\epsilon^2}$ and the second one is due to by *system dimension.*
These limits can be explained in this way : in order to value more oscillating wave functions we need more precision and so a smaller and smaller ϵ ,on the other hand ,we need also that *effective length* be much bigger than *typical length.*
Knowing that harmonic oscillator eigenvalues in one dimension are described by :

$$E_n = (n + \frac{1}{2})\hbar\omega \tag{6}$$

we have $n_{upper} \simeq \frac{1}{\omega\epsilon^2}$. This estimate is in accordance with continuous case : when $\epsilon \to 0$ and $n_{upper} \to \infty$ as should be .

Fixing $\hbar = 1$ and 2m=1 ,after discretization procedure , the hamiltonian's system becomes a 2L+1 real symmetric square matrix H where :

$$H_{kl} = \begin{cases} \frac{+2}{\epsilon^2} + \frac{1}{4}\omega^2 {x_l}^2 & l = k \\ \frac{-1}{\epsilon^2} & l = k+1, l = k-1 \\ 0 & \text{otherwise} \end{cases} \tag{7}$$

so harmonic oscillator equation becomes :

$$\sum_l H_{kl}\psi_l^{(n)} = E_n\psi_k^{(n)} \tag{8}$$

and *typical length* $x_0 = \sqrt{\frac{2}{\omega}}$

3 Code development

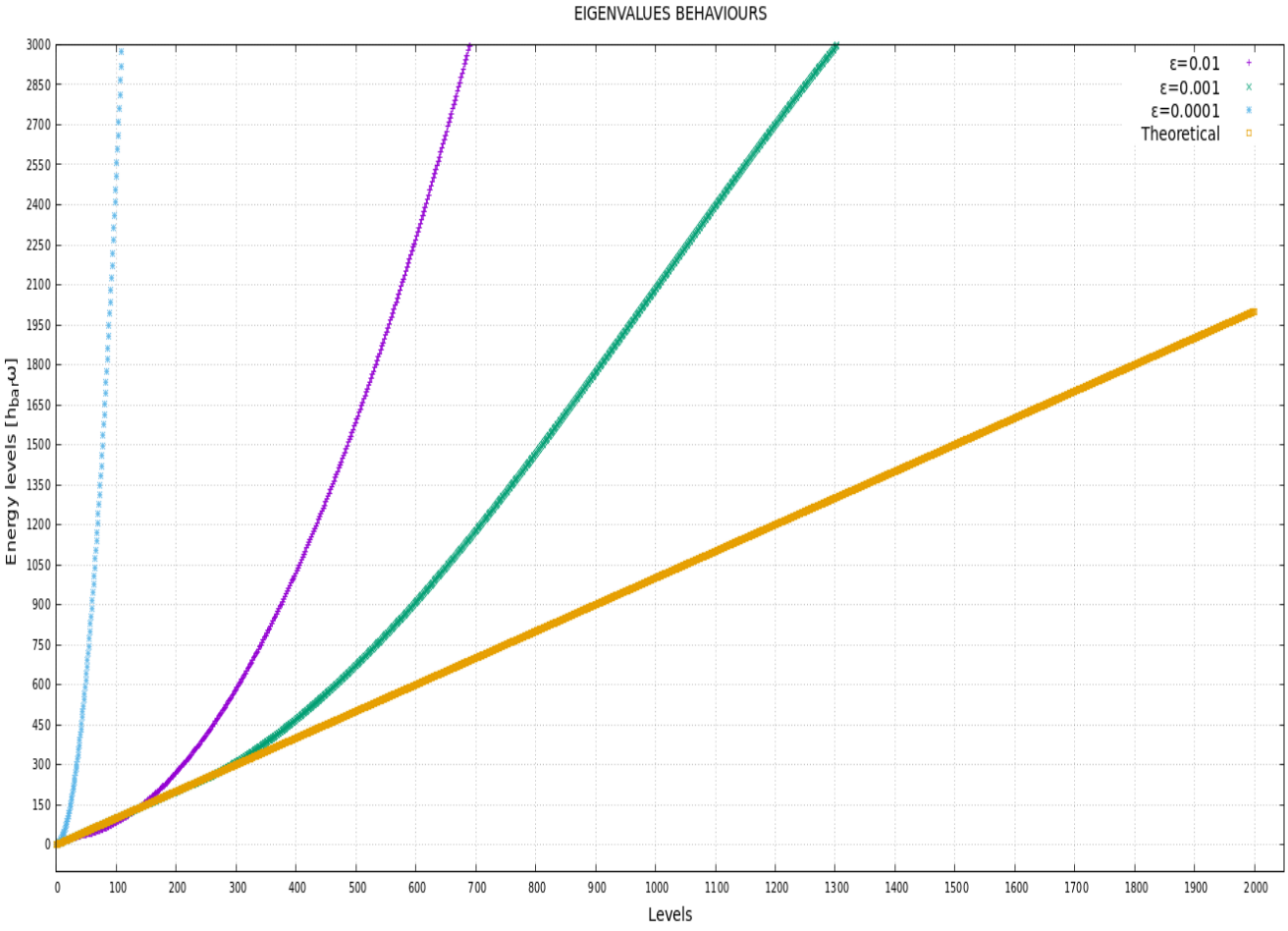
My code is composed by two units program : one *module* and one *main program.*

- MODULE ***Harmonic Oscillator***: here we define harmonic oscillator hamiltonian discretized matrix and the time(in seconds) needful to execute this aim.

- PROGRAM ***MAIN*** : here we define useful parameters like L,ω and ϵ and we apply DSYEV lapack function in order to compute eigenvalues and normalized ortogonal eigenfunctions and write them on different files.
  DSYEV at place of CHEEV function because we are sure,at the beginning,that both E_n and ψ_n are reals .
  In order to check if eigenvectors are really normalized and ortogonal between them a simple check is implemented : computed eigenfunctions and put them in a matrix A , a matrix-matrix multiplication with A transpose must gives us identity matrix.

4 Results

In the following we'll show our results achieved both using fortran code and GNUPLOT software fixing $\omega = 10^3$ and L=10^3.



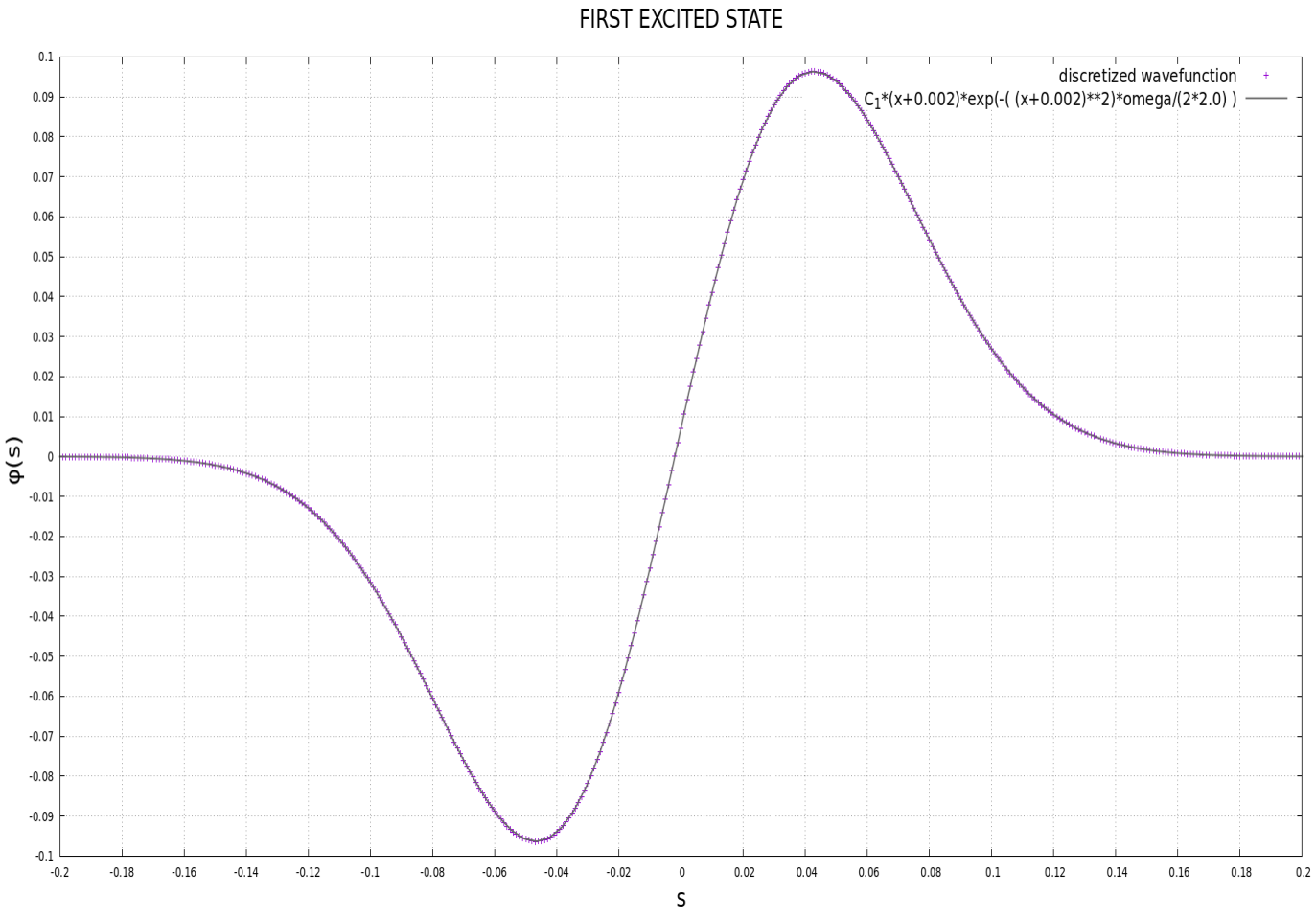
As shown above using different ϵ values we obtain different eigenvalues behaviours.
Theoretical energy limits and *effective lengths* are:

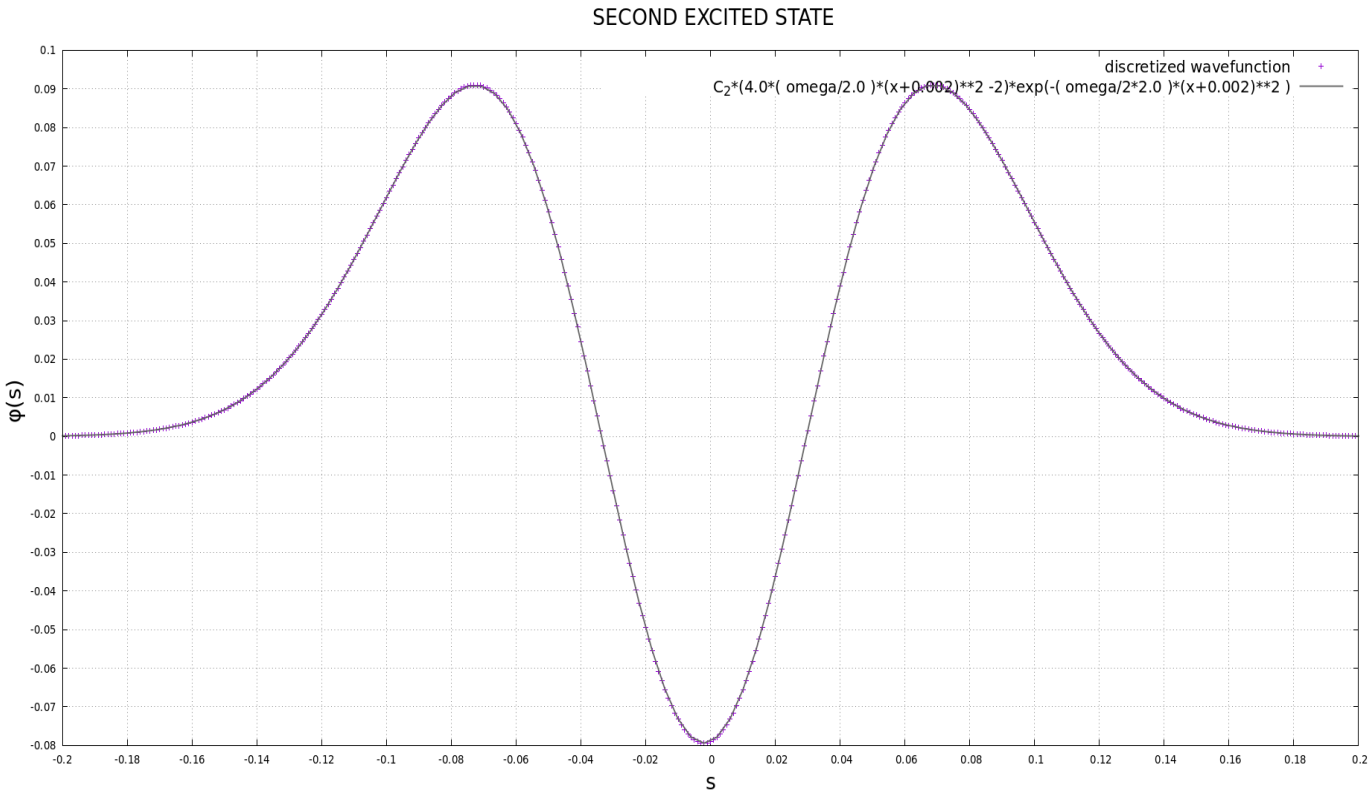
- for $\epsilon = 0.01$: $n_{upper} \simeq \frac{1}{\omega\epsilon^2} \simeq 10^1$ and $L' \simeq \epsilon \mathrm{L} \simeq 10$
- for $\epsilon = 0.001$: $n_{upper} \simeq \frac{1}{\omega\epsilon^2} \simeq 10^3$ and $L' \simeq \epsilon \mathrm{L} \simeq 1$
- for $\epsilon = 0.0001$: $n_{upper} \simeq \frac{1}{\omega\epsilon^2} \simeq 10^5$ and $L' \simeq \epsilon \mathrm{L} \simeq 0.1$

For $\epsilon = 0.0001$ limits are not respected because L' is the same magnitude of $x_0 \simeq 0.045$ and we know that $x_0 << L'$.

For $\epsilon = 0.01$ we notice a little divergence from theoretical behaviour that it begins from $\simeq$ 50th level and it can be in accordance with 10^1 order of magnitude.

Finally for $\epsilon = 0.001$ theoretical limits are respected if we consider that n_{upper} is indeed an *upper limit* but in general n_{max} reached by algorithm is equal or lower than previous one.
In the following first and second state's wavefunctions are shown





5 Self-evaluation

Dealing about correctness's code and accurate discretization we suppose,seeing results, that everything works properly. Instead dealing about its stability ,we think it much depends by parameters proved : scaling down from $\epsilon = 10^{-2}$ to $\epsilon = 10^{-3}$ we observe an improvement in accurateness of eigenvalues found but on the other hand from $\epsilon = 10^{-3}$ to $\epsilon = 10^{-4}$ results get worse.
To generalize this code in order to face up harmonic oscillator problem in more dimensions or adapt it taking into account different potentials shouldn't require an huge effort. Each code running takes only few seconds and we used DSYEV instead of CHEEV lapack function because in this way time spending is lower.