Solving 1d Harmonic Oscillator by DVR Method

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1 Introduction :

Discrete Variable Representation or, *DVR* Method is the representation of discrete values of coordinate system to numerically solve the system by discretization of continuous parameters describe the system. To be more precise, the DVR method is a representation whose associated basis functions are localized about the discrete values of the approximation : coordinate operators are diagonal in this representation and have approximate values at DVR points [4]. Therefore we can say that DVR method utilizes the transformation between a finite discrete basis and the finite grid that spans the region of system in which we are interested.
Example : Numerical solution of the wavefunctions of a bound potential in the position representation requires discretizing and truncating region of space that is spanned by Hilbert space (infinite dimensional). Considering the Harmonic Oscillator wavefunctions, the real continuous basis $\delta(x)$ of Hamiltonian eigenstates will be represented in grid basis $\theta_{(i)}$ approximately. There will be two basis sets:

1. Eigenbasis ϕ
2. Grid basis θ

These two basis sets are connected through the unitary transformation :

$$\Phi^{\dagger}\phi(x) = \theta(x)\phi\theta(x) = \phi(x)$$

The N eigensates will be correspondent to N discrete points in the grid basis maintaining the properties of completeness and orthogonal in both bases. Hence, the wavefunctions that we will get by implementing the algorithm will be constructed from the Hamiltonian in the eigenbasis. Here, we will consider the Fourier Grid Hamiltonian Method as a special case of Discrete Variable Method.

Fourier Grid Hamiltonian (FGH) is a numerical method to calculate the bound state eigenvalues and eigenstates of Schrödinger Equation. The FGH method is derived from discrete Fourier Transform algorithm. The working principle of this algorithm is to evaluating the potential at certain grid points and directly evaluating the amplitude of the eigenstates at those same grid points. In particular the Fourier Grid Hamiltonian method is simpler and the accuracy is high. The method can be applied for different dimensional system and also it relies on the fact that : **the kinetic energy operator is represented in momentum space, while the potential energy factor will be represented in coordinate space.**

$$H = T(\hat{p}) + V(\hat{x})$$

In DVR basis :

$$H^{DVR} = \Phi H \Phi$$

Then the Hamiltonian matrix will be diagonalized.

In 1989, Marston et al. proposed the Fourier Grid Hamiltonian Method to solve the time-independent Schrodinger equation that is to finding the eigensates and the corresponding eigenvalues.

2 FGH Method for Solving 1d Harmonic Oscillator :

The 1d Schrödinger Equation is :

$$\hat{H}|\Psi\rangle = (\frac{\hat{P}^2}{2m} + V(\hat{X})|\Psi\rangle = E|\Psi\rangle \tag{1}$$

Here $\hat{P}$ is the momentum operator defined as :

$$\hat{P}|k\rangle = \hbar k|k\rangle \tag{2}$$

Here $\hat{X}$ is the momentum operator defined as :

$$\hat{X}|x\rangle = x|x\rangle \tag{3}$$

The orthonormality conditions are written as :

$$
\begin{aligned}
\langle x'|x\rangle &= \delta(x'-x) \\
\langle k'|k\rangle &= \delta(k'-k)
\end{aligned}
\tag{4}
$$

From Fourier transformation and using 4
we get,

$$\langle k|x\rangle = \frac{1}{2\pi} exp(-ikx) \tag{5}$$

Now,

$$
\begin{aligned}
\langle x|\hat{H}|x'\rangle &= \langle x|\frac{\hat{P}^2}{2m}|x'\rangle + \langle x|V(\hat{X})|x'\rangle \\
&= \int_{-\infty}^{\infty} dk' \int_{-\infty}^{\infty} dk'' \langle x|k'\rangle\langle k'|\frac{\hat{P}^2}{2m}|k''\rangle\langle k''|x'\rangle + V(\hat{X})\delta(x-x') \\
&= \int_{-\infty}^{\infty} dk' \int_{-\infty}^{\infty} dk'' \langle x|k'\rangle \frac{(\hbar k')^2}{2m}\delta(k''-k')\langle k''|x'\rangle + V(\hat{X})\delta(x-x') \\
&= \int_{-\infty}^{\infty} dk' \frac{(\hbar k')^2}{2m}\langle x|k'\rangle\langle k'|x'\rangle + V(\hat{X})\delta(x-x')
\end{aligned}
$$

The completeness relation is :

$$\int_{-\infty}^{\infty} dk'|k'\rangle\langle k'| = \hat{I}$$

Therefore,

$$\langle x|\hat{H}|x'\rangle = \frac{(1)}{2\pi}\int_{-\infty}^{\infty} dk' T_{k'} exp\{ik'(x-x')\} + V(\hat{X})\delta(x-x') \tag{6}$$

$$\tag{7}$$

Where, Kinetic Energy, $T_{k'} = \dfrac{(\hbar k')^2}{2m}$

Now, the discretization for Fourier Grid Hamiltonian method is done as follows :

- We have to choose a finite grid .
- Then we have to specify the grid size.

- We will have the discretization parameters : Δx and n.

The meaning of the grid is to definie the continuous variable to discrete variable in such a way that the numerical solution will have the highest accuracy. To express the statement mathematically we can write :

$$x, \forall x \in \mathbb{R} \ \mapsto \ x_i, \forall \{i\} \in \{-n, -n+1, ...0, ..., n-1, n\}$$

Where, x_i = iΔx and N = 2n+1
The size of the grid is = NΔx such that the corresponding wavenumber will be $\Delta k = \dfrac{2\pi}{N\Delta x}$
Now we have to write the integral form as discrete summation :

$$\int_{-\infty}^{\infty} \mapsto \Sigma_{i=-n}^{n} \Delta x and \ \delta(x_i - x_j) \mapsto \frac{1}{\Delta x}\delta_{ij}$$

$$\int_{-\infty}^{\infty} dx' \langle x|\hat{H}|x'\rangle |\Psi(x)\rangle = E|\Psi(x)\rangle \tag{8}$$

In the discrete form the above eqn. will be :

$$\Sigma_{i=-n}^{n} \Delta x^2 \langle x_j|\hat{H}|x_i\rangle |\Psi(x_i)\rangle = E|\Psi(x_j)\rangle \tag{9}$$

Comparing the equation with

$$\hat{H}|\Psi\rangle = E|\Psi\rangle$$

We can understand that H the matrix which has dimension of N$\times$N

$$\langle x|\hat{H}|x'\rangle = \frac{1}{2\pi}\int_{-\infty}^{\infty} dk' T_{k'} exp\{ik'(x - x')\} + V(\hat{X})\delta(x - x')$$

By discretization of the above equation we get,

$$\langle x_j|\hat{H}|x_i\rangle = \frac{1}{2\pi}\Sigma_{i=-n}^{n} \Delta k T_{k_i} exp\{ik_i(x_j - x_i)\}\frac{1}{\Delta x}\delta_{ij} + V(x_i)\frac{1}{\Delta x}\delta_{ij} \tag{10}$$

Now, using the expression of $\Delta k = \dfrac{2\pi}{N\Delta x}$

$$\Delta x \langle x_j|\hat{H}|x_i\rangle = \frac{1}{N}\Sigma_{i=-n}^{n} T_{k_i} exp\{ik_i(x_j - x_i)\}\delta_{ij} + V(x_i)\delta_{ij} \tag{11}$$

Now using the expression for kinetic energy, $T_k = \frac{(\hbar k)^2}{2m} \Rightarrow T_{-k} = T_k$
and $\frac{e^{i\theta} - e^{-i\theta}}{2} = \cos\theta$
Therefore exploiting these equations we get,

$$\Delta x \langle x_j|\hat{H}|x_i\rangle = \frac{1}{N}\Sigma_{i=-n}^{n} T_{k_i}\ cos\{ik_i(x_j - x_i)\}\delta_{ij} + V(x_i)\delta_{ij} \tag{12}$$

3 Program Written for DVR Method :

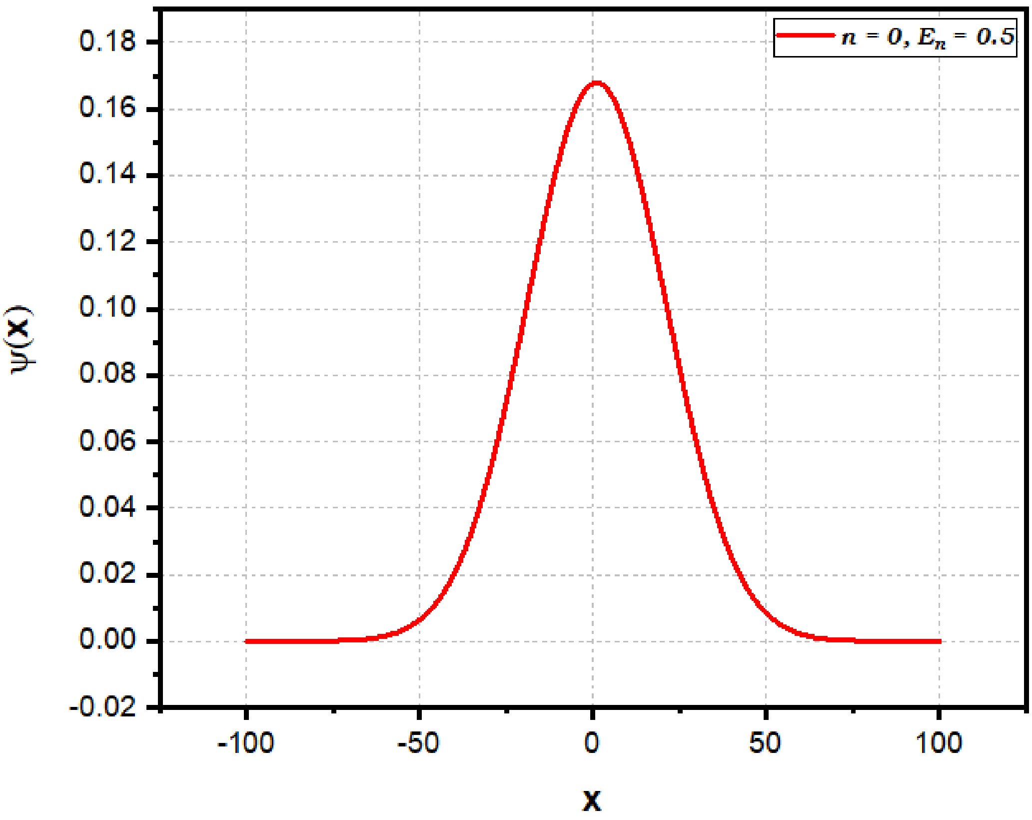
code for DVR
The program file is attached in the link above.

4 Numerical Data for Eigenvalues & the Eigenstates :

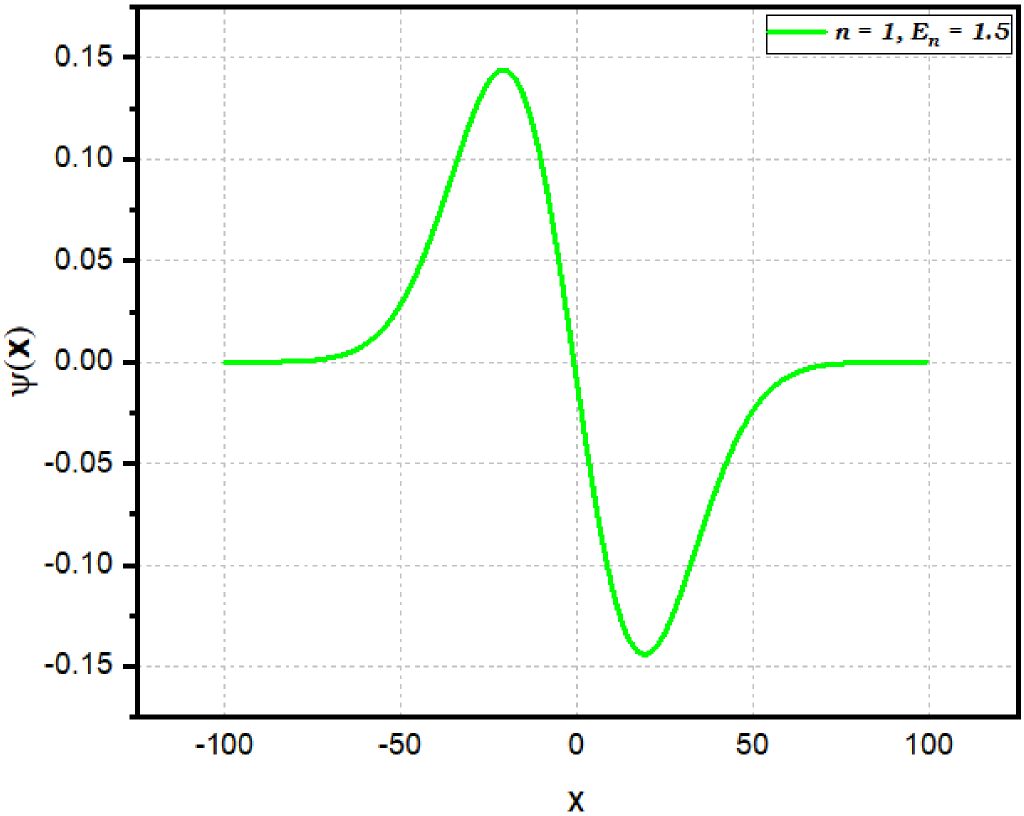
n	N = 50	N = 100	N = 150	N = 200	Accurate Eigenvalues
0	0.5	0.5	0.5	0.5	0.5
1	1.5	1.5	1.5	1.5	1.5
2	2.5	2.5	2.5	2.5	2.5
3	3.5	3.5	3.5	3.5	3.5
4	4.5	4.49999	4.5	4.5	4.5
5	5.5	5.50008	5.5	5.5	5.5
6	6.5	6.49943	6.5	6.5	6.5
7	7.5	7.5025	7.5	7.5	7.5
8	8.5	8.48767	8.5	8.5	8.5
9	9.5	9.53236	9.5	9.5	9.5
10	10.5	10.38657	10.5	10.5	10.5
11	11.5	11.695	11.5	11.5	11.5
12	12.5	12.17349	12.5	12.5	12.5
13	13.5	14.15382	13.5	13.5	13.5
14	14.5	14.33982	14.5	14.5	14.5
15	15.5	17.00411	15.5	15.5	15.5
16	16.5	17.0852	16.5	16.5	16.5
17	17.5	20.26533	17.50002	17.5	17.5
18	18.5	20.30946	18.49992	18.5	18.5
19	19.5	23.93421	19.50027	19.5	19.5
20	20.5	23.96223	20.49897	20.5	20.5

Table : **EigenValues for Different Grid Points**

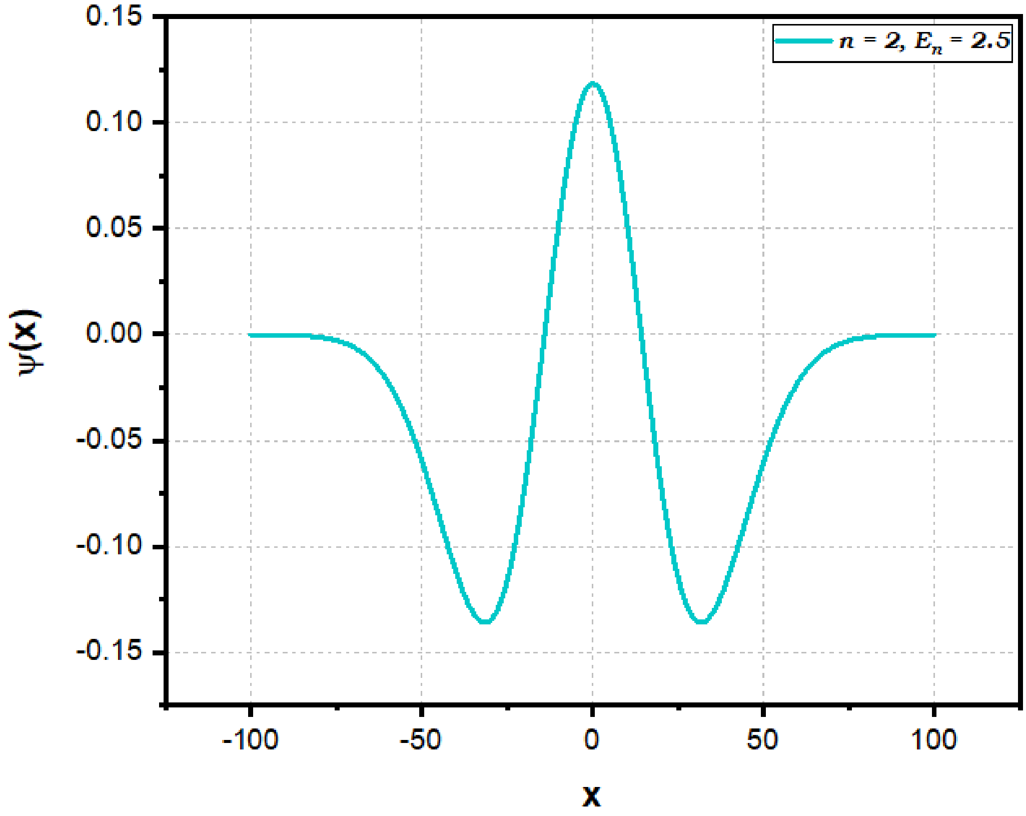
4.1 Eigenstate Corresponding to n = 0



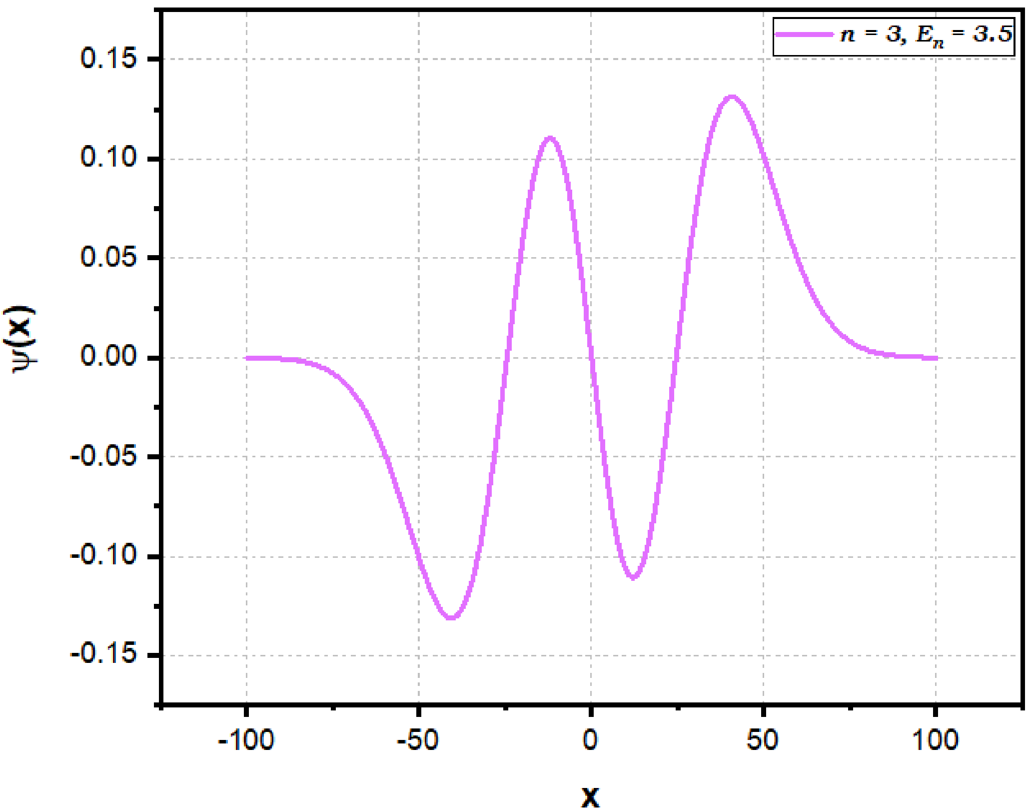
4.2 Eigenstate Corresponding to n = 1



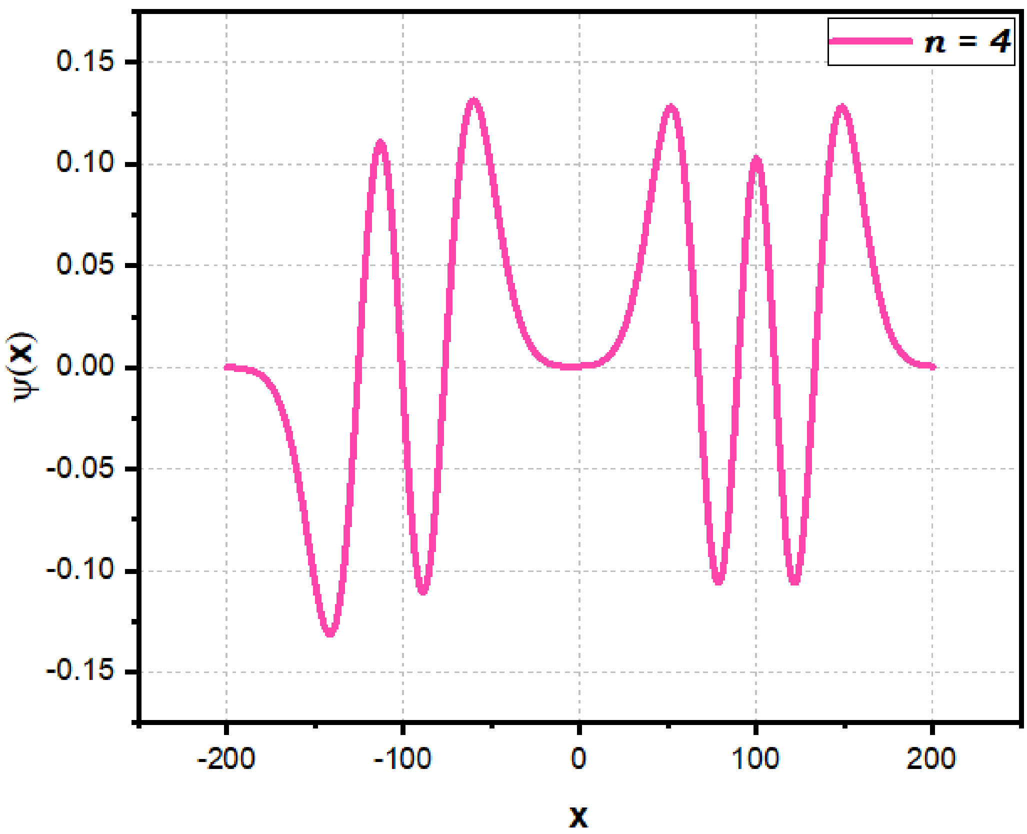
4.3 Eigenstate Corresponding to n = 2



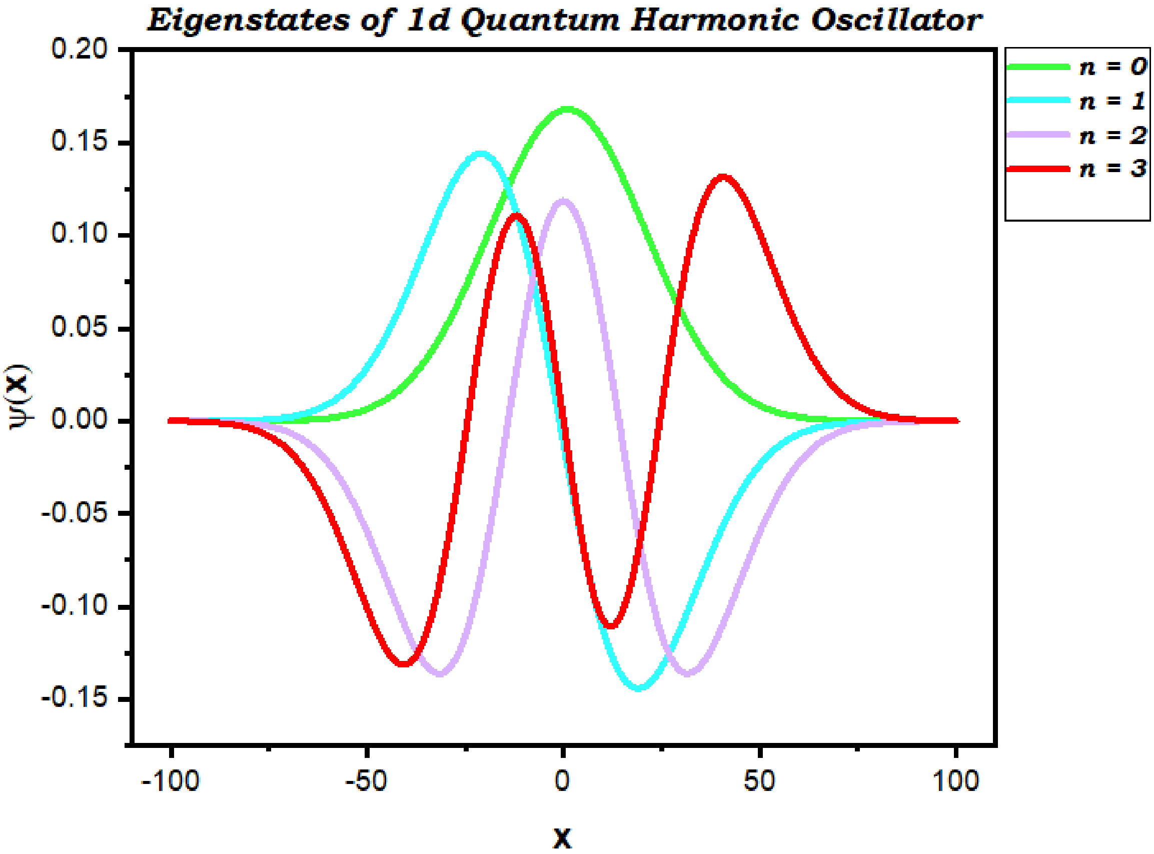
4.4 Eigenstate Corresponding to n = 3



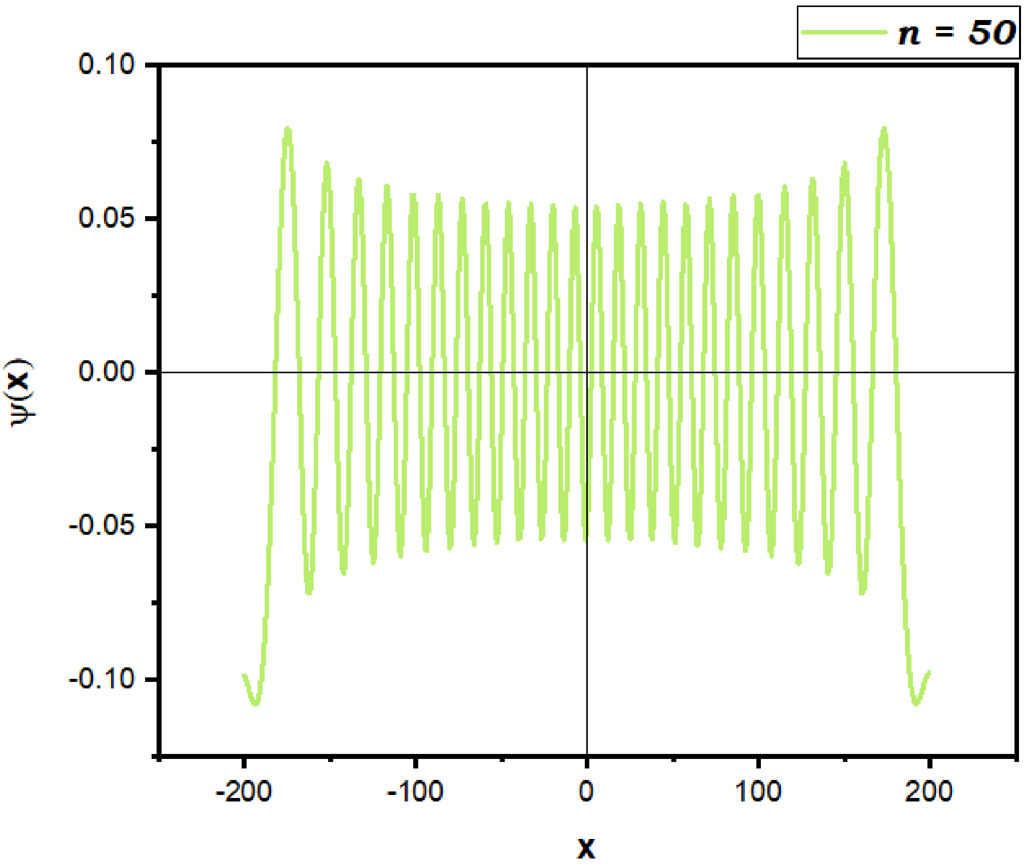
4.5 Eigenstate Corresponding to n = 4



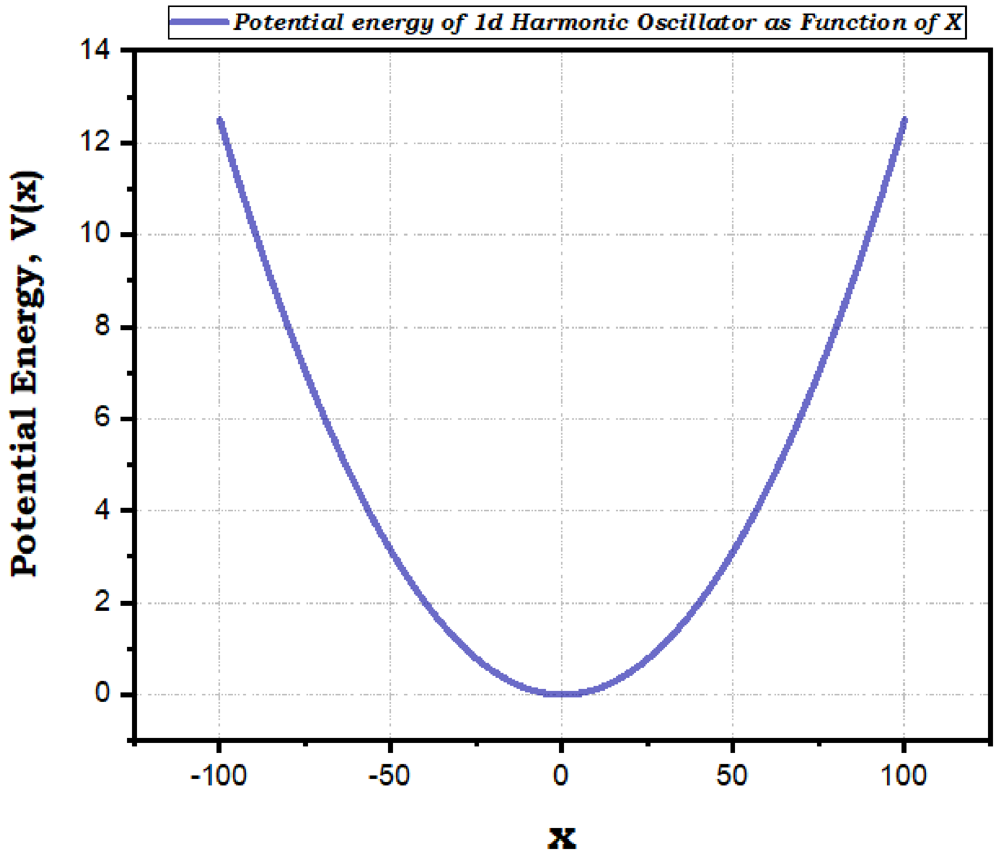
4.6 All Eigenstates



4.7 Eigenstate Corresponding to n = 50



4.8 Potential V(x) of 1D Harmonic Oscillator



5 Conclusion :

From the result that we got by implementing the Fourier Grid Hamiltonian Method is indicating the dependence of accuracy of the method on two parameters :

1. Number of Grid Points (N)
2. Uniform Spacing between the Grid Points (Δx)

And we have seen for a particular value of Δx, if the grid points are increased in number the accuracy increases.

6 References :

1. C. C. Marston and G. G. Balint-Kurti, J. Chem. Phys. 91, 3571 (1989).

2. G. G. Balint-Kurti, C. L. Ward, and C. C. Marston, Comp. Phys. Commun. 67, 285 (1991).

3. M. Feit, J. Fleck, and A. Steiger. Solution of the Schrödinger equation by a spectral method. Journal of Computational Physics, 47(3):412–433, 1982.