Date : / /

2020PHY1216

LAB ASSIGNMENT - 13

THEORY

The potential is given by :-

$$V(x) = \frac{1}{2} kx^2 + bx^3 \quad ; \quad k = \mu\omega^2$$

(a)

Since, we know that the time Independent Schrodinger Equation is given by :-

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} + V(r)\,u = Eu$$

$$\text{or} \quad \frac{d^2u}{dr^2} + \frac{2m}{\hbar^2}\left(E - V(r)\right)u = 0$$

$$\therefore \frac{d^2u}{dr^2} + \frac{2m}{\hbar^2}\left(E - \frac{1}{2}kr^2 - \frac{1}{3}br^3\right) = 0 \quad \text{—} \ ①$$

Now, for making r & E dimensionless.
Let :-

$$r = r_0\xi \quad \& \quad E = E_0 E$$

Now, $\because$

$$\frac{du}{dr} = \frac{du}{d\xi}\left(\frac{d\xi}{dr}\right)$$

2020 PHY1216

$$\frac{du}{dr} = \frac{1}{r_0}\frac{du}{d\xi}$$

Again differentiating w.r.t 'r' :-

$$\left[\frac{d^2u}{dr^2} = \frac{1}{r_0^2}\frac{d^2u}{d\xi^2}\right]$$

putting this in ① :-

$$\frac{d^2u}{d\xi^2} + \frac{2m r_0^2}{\hbar^2}\left[\varepsilon_0 E - \frac{1}{2}k(r_0\xi)^2 - \frac{1}{3}b(r_0\xi)^3\right]u = 0$$

$$\Rightarrow \frac{d^2u}{d\xi^2} + \frac{2m}{\hbar^2}\left[\varepsilon_0 E r_0^2 - \frac{1}{2}k r_0^4\xi^2 - \frac{1}{3}b r_0^5\xi^3\right]u = 0$$

$$\Rightarrow \frac{d^2u}{d\xi^2} + \left[\frac{2m\varepsilon_0 r_0^2}{\hbar^2}E - \frac{mk r_0^4}{\hbar^2}\xi^2 - \frac{2}{3\hbar^2}mb r_0^5\xi^3\right]u = 0$$

— ②

for finding these terms in dimensionless form we will equate the coefficients of ξ^2, E & ξ^5 equals to 1 one by one.

$$\therefore \frac{mk r_0^4}{\hbar^2} = 1$$

$$\left[r_0 = \left(\frac{\hbar^2}{mk}\right)^{1/4}\right]$$

Page No.
Date :

2020 PHY1216

$$\frac{2m r_0^2 \, \varepsilon_0}{\hbar^2} = 1$$

$$\varepsilon_0 = \frac{\hbar^2}{2m r_0^2}$$

$$= \frac{\hbar^2}{2m} \frac{(mk)^{1/2}}{(\hbar^2)^{1/2}}$$

$$\varepsilon_0 = \frac{\hbar}{2m} (mk)^{1/2}$$

$$\left[\varepsilon_0 = \frac{\hbar}{2}\sqrt{\frac{k}{m}} = \frac{\hbar}{2}\omega \right]$$

Now, with coefficients of ξ^5 :-

$$\Rightarrow \frac{2mb}{3\hbar^2} r_0^5 = 1$$

$$\Rightarrow \frac{2mb}{3\hbar^2} \left(\frac{\hbar^2}{mk} \right)^{5/4}$$

$$= \frac{2mb \cdot \cancel{\hbar^2}\, r_0}{mu \cdot 3\cancel{\hbar^2}}$$

$$= \frac{2}{3} \frac{b r_0}{K}$$

Let, $\left[\frac{b r_0}{k} = \alpha \right]$

2020 PHY1216

Page No.
Date : / /

Putting all these values in equ ② :-

$$\frac{d^2u}{d\xi^2} + \left[\varepsilon - \xi^2 - \frac{2}{3}\frac{b\sigma}{k}\xi^3\right]u = 0$$

$$\boxed{\frac{d^2u}{d\xi^2} + \left[\varepsilon - \left(\xi^2 + \frac{2}{3}\alpha\xi^3\right)\right]u = 0}$$

dimensionless potential $\rightarrow \left[\xi^2 + \frac{2\alpha}{3}\xi^2\right] \rightarrow V(\xi)$

Now, defining ε :-

$$\therefore \varepsilon = \frac{E}{E_0} = \frac{(n+1/2)\cancel{\hbar\omega}}{\cancel{\hbar\omega}/2}$$

$$\left[\varepsilon = 2n+1\right], n = 0, 1, 2, \ldots$$

1 Discussion

The states in these graphs are used as in numerical method so read 0^{th} state as 1^{st}

1. The table below shows the Eigen Values for first ten excited states for different values of **alpha** mentioned in each table

The Eigen values for alpha=0

	Eigen Values	Perturbted Eigen value
0	32.175281	32.176082
1	96.524241	96.528247
2	160.870000	160.880411
3	225.212622	225.232575
4	289.552700	289.584740
5	353.894373	353.936904
6	418.259665	418.289069
7	482.738729	482.641233
8	547.613596	546.993397
9	613.547575	611.345562

The Eigen values for alpha=1

	Eigen Values	Perturbted Eigen value
0	-1072.544034	-56.308144
1	-577.702207	-474.597212
2	-253.253015	-1375.527514
3	-45.021813	-2759.099049
4	27.815192	-4625.311817
5	78.965863	-6974.165818
6	147.433537	-9805.661051
7	227.226851	-13119.797518
8	315.290667	-16916.575218
9	410.529169	-21195.994151

Figure 1:

The Eigen values for alpha=0.1

	Eigen Values	Perturbted Eigen value
0	32.075790	31.291240
1	95.875183	90.816992
2	159.101208	145.516332
3	221.730145	195.389259
4	283.751247	240.435774
5	345.250097	280.655877
6	406.680726	316.049567
7	469.194478	346.616846
8	534.322584	372.357711
9	603.084011	393.272165

The Eigen values for alpha=0.01

	Eigen Values	Perturbted Eigen value
0	32.174298	32.167234
1	96.517894	96.471134
2	160.852927	160.726770
3	225.179463	224.934142
4	289.498140	289.093250
5	353.813421	353.204094
6	418.148996	417.266674
7	482.601010	481.280989
8	547.465423	545.247041
9	613.422185	609.164828

Figure 2:

The Eigen values for alpha=0.001

	Eigen Values	Perturbted Eigen value
0	32.175271	32.175994
1	96.524177	96.527675
2	160.869830	160.878875
3	225.212291	225.229591
4	289.552155	289.579825
5	353.893564	353.929576
6	418.258559	418.278845
7	482.737351	482.627631
8	547.612113	546.975934
9	613.546318	611.323755

The Eigen values for alpha=0.0001

	Eigen Values	Perturbted Eigen value
0	32.175281	32.176081
1	96.524240	96.528241
2	160.869999	160.880396
3	225.212619	225.232546
4	289.552695	289.584691
5	353.894365	353.936831
6	418.259654	418.288966
7	482.738715	482.641097
8	547.613581	546.993223
9	613.547562	611.345344

Figure 3:

2. These are the plots of the eigen values with states for different alpha

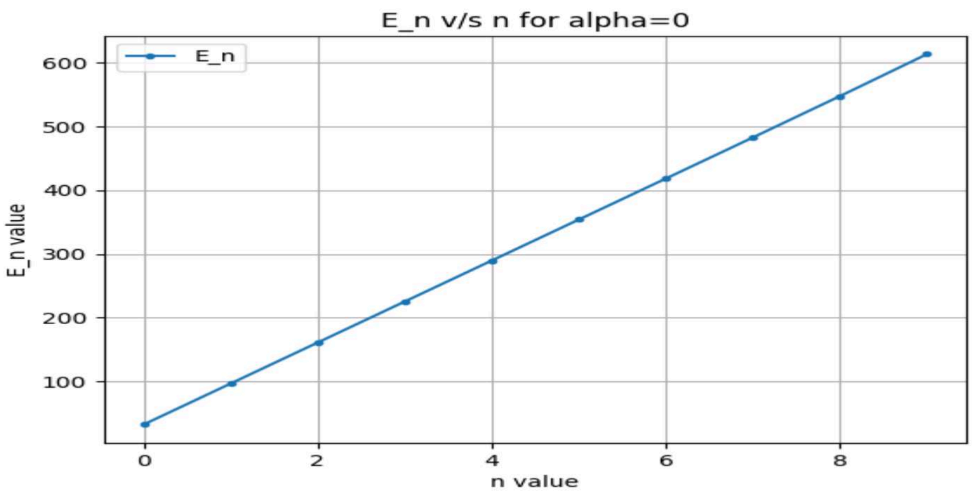

Figure 4:

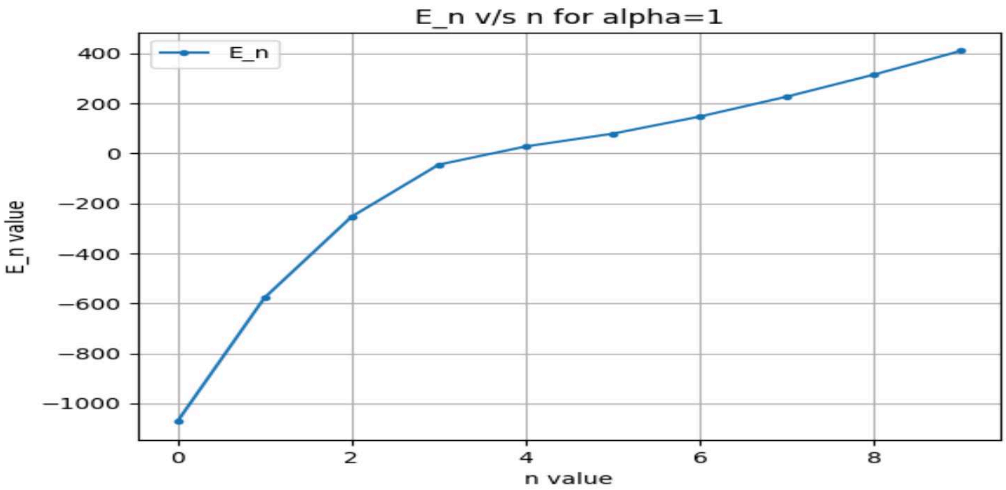

Figure 5:

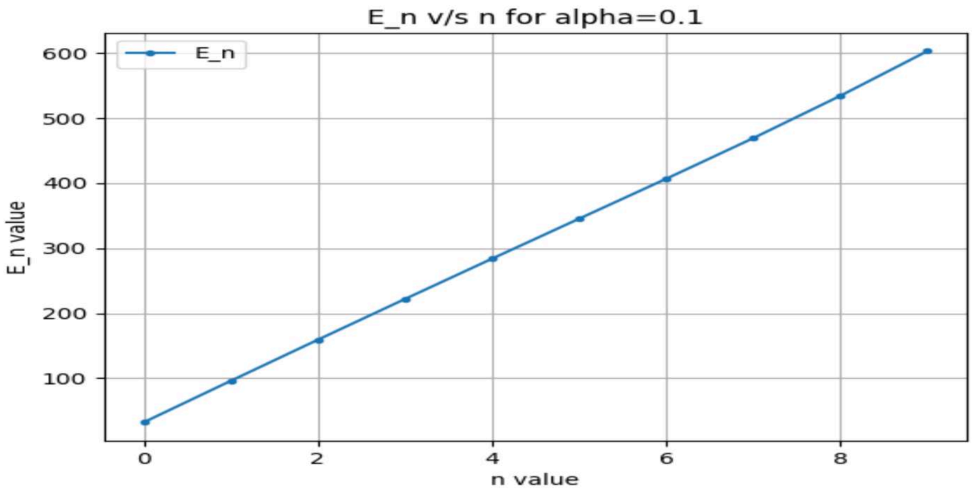

Figure 6:

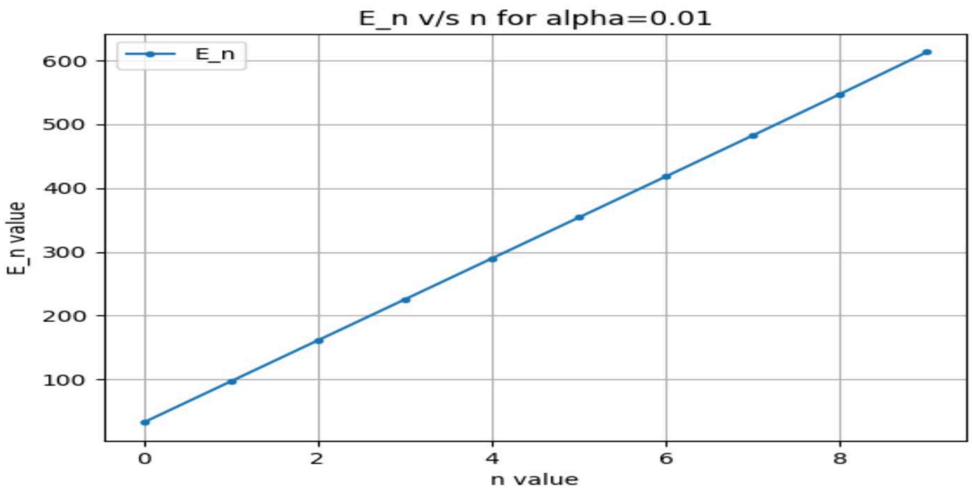

Figure 7:

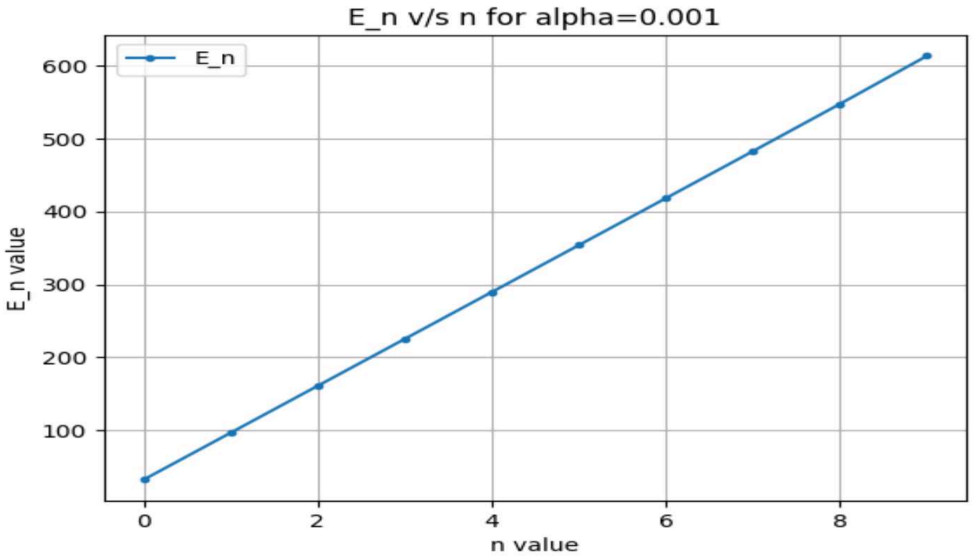

Figure 8:

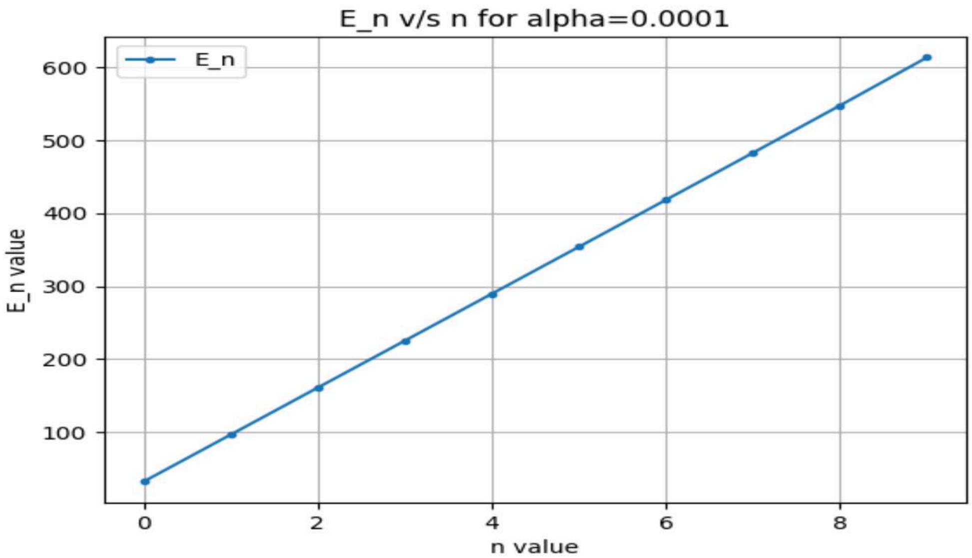

Figure 9:

3. Here I am plotting the Radial wavefunction for different value of ratio(α) given in the assignment .

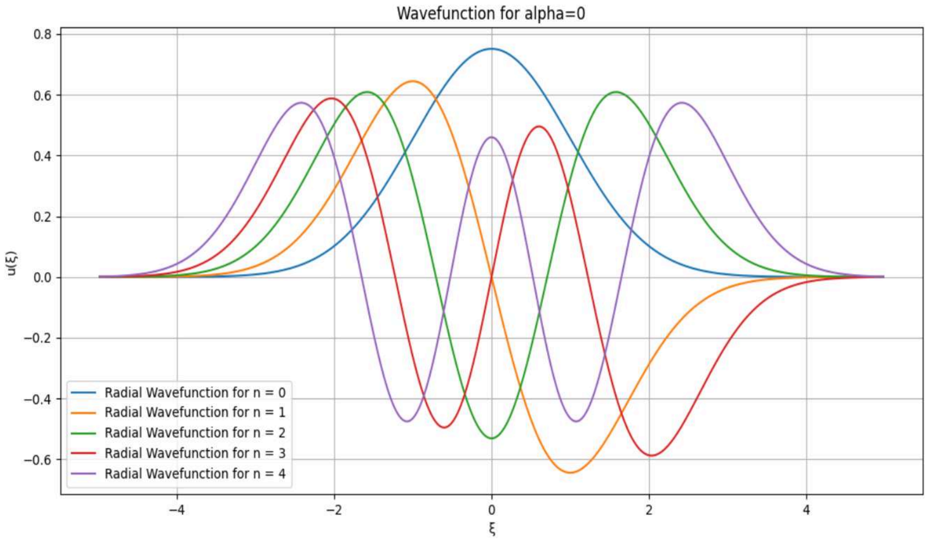

Figure 10:

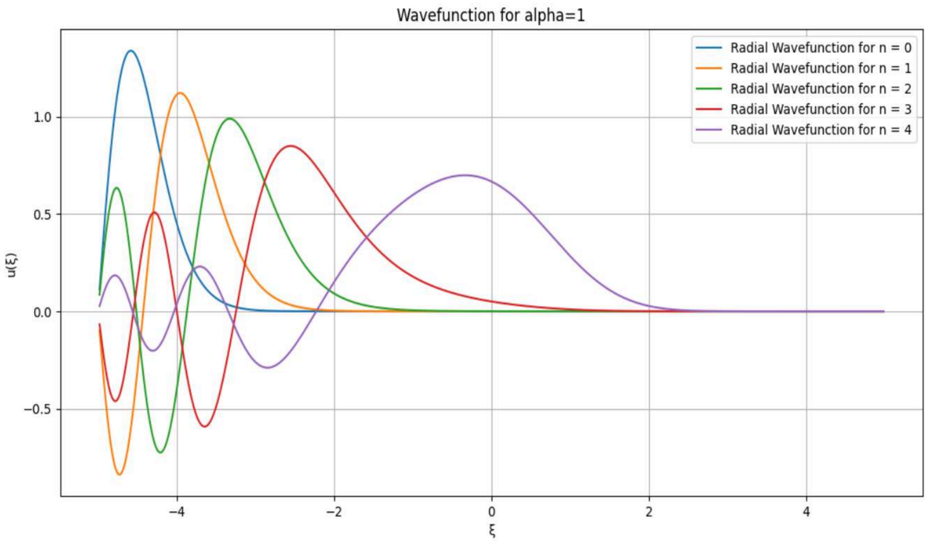

Figure 11:

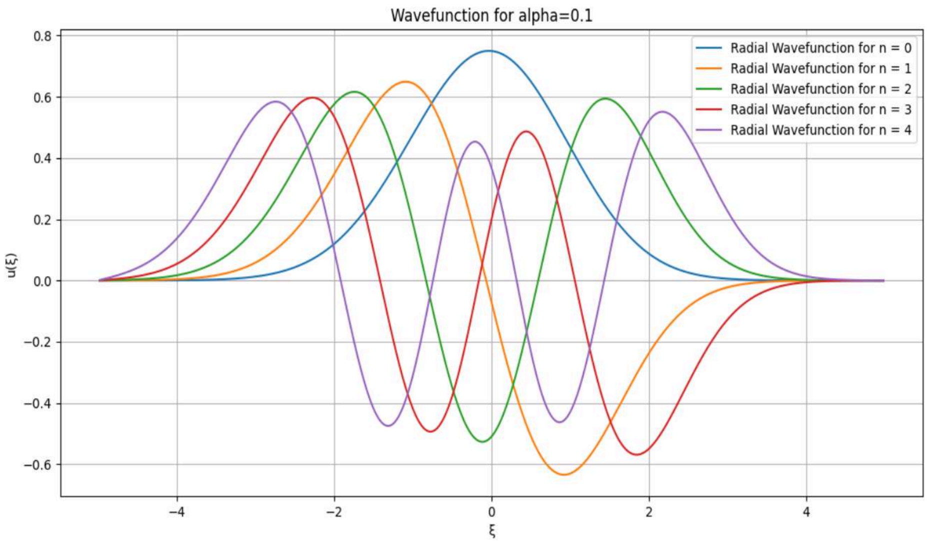

Figure 12:

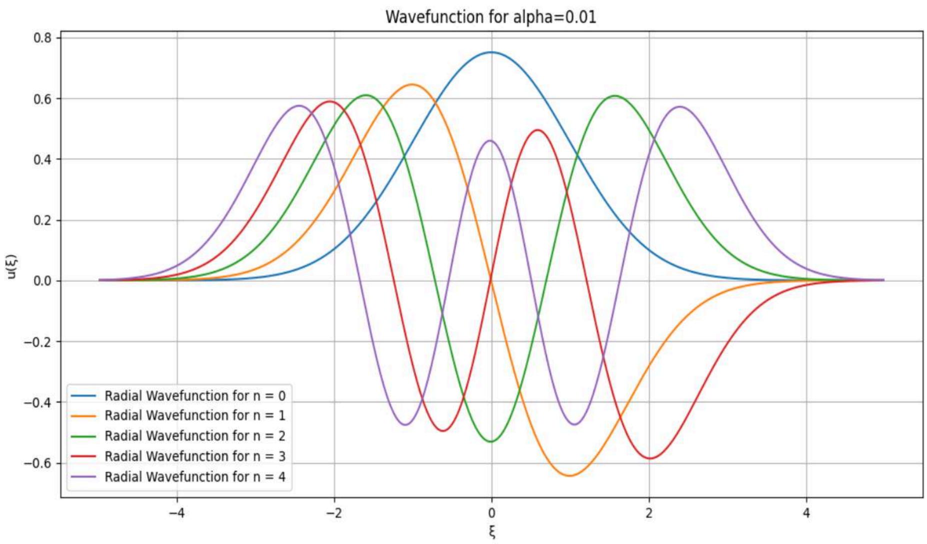

Figure 13:

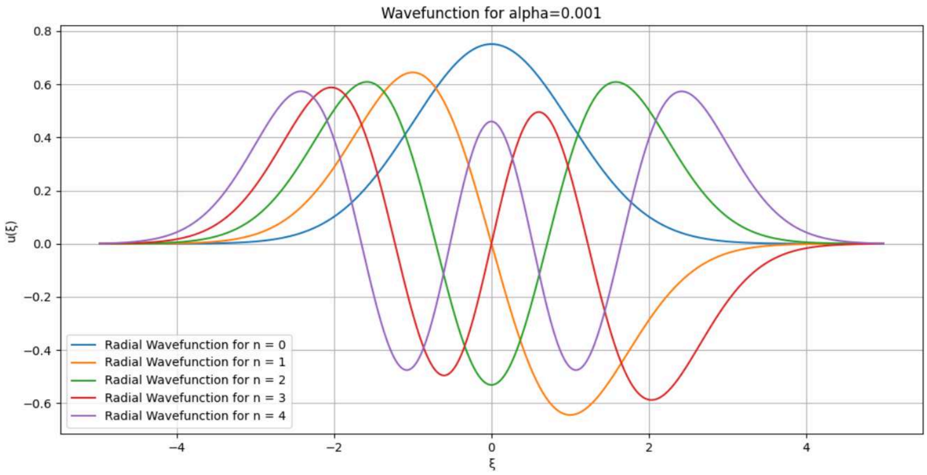

Figure 14:

4. This plot shows Probability Density of the waveform plotted above.

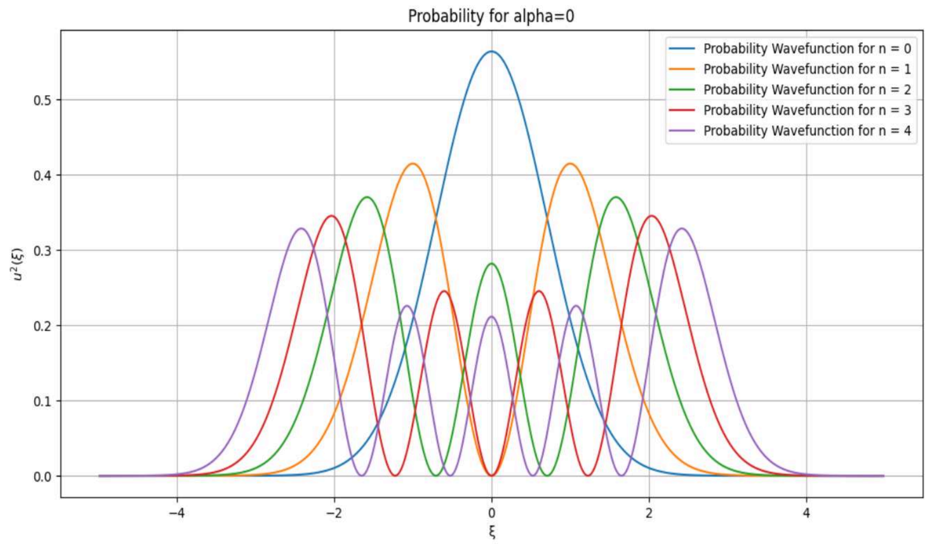

Figure 15:

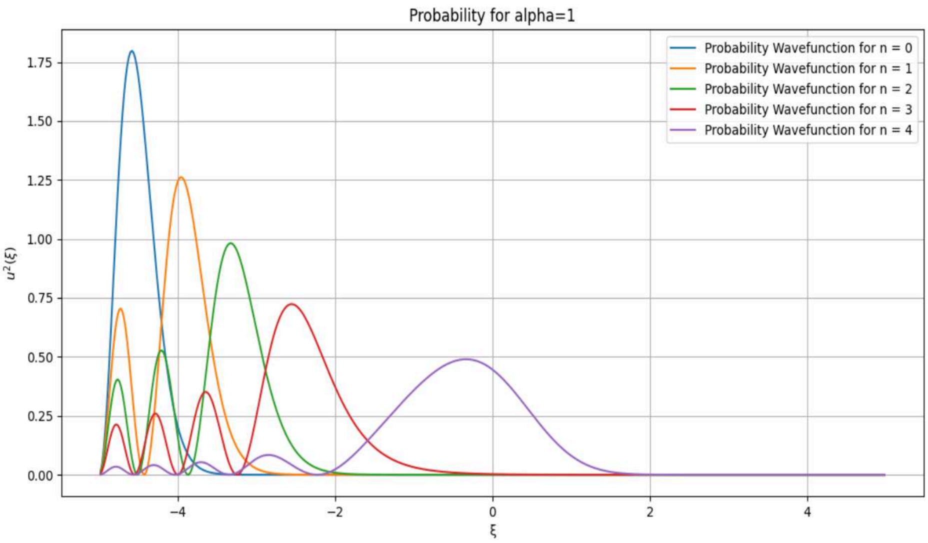

Figure 16:

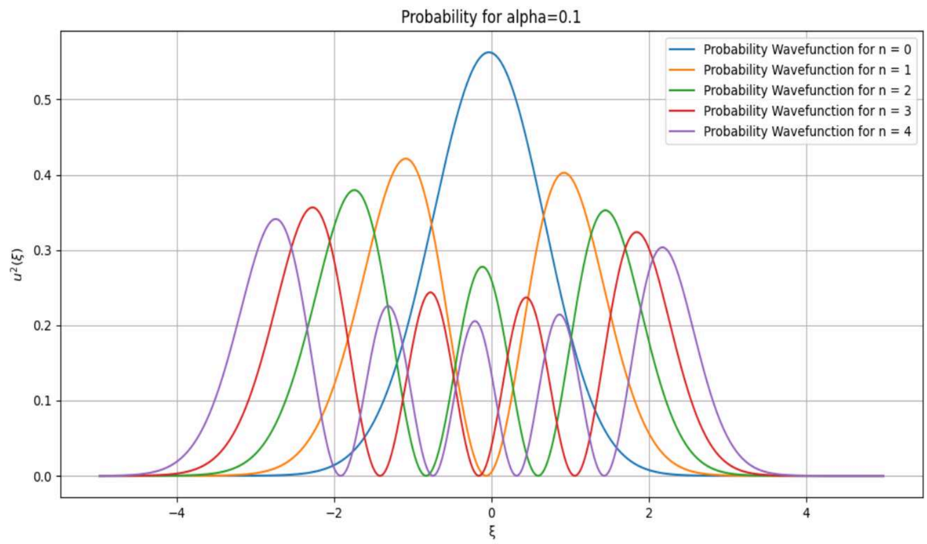

Figure 17:

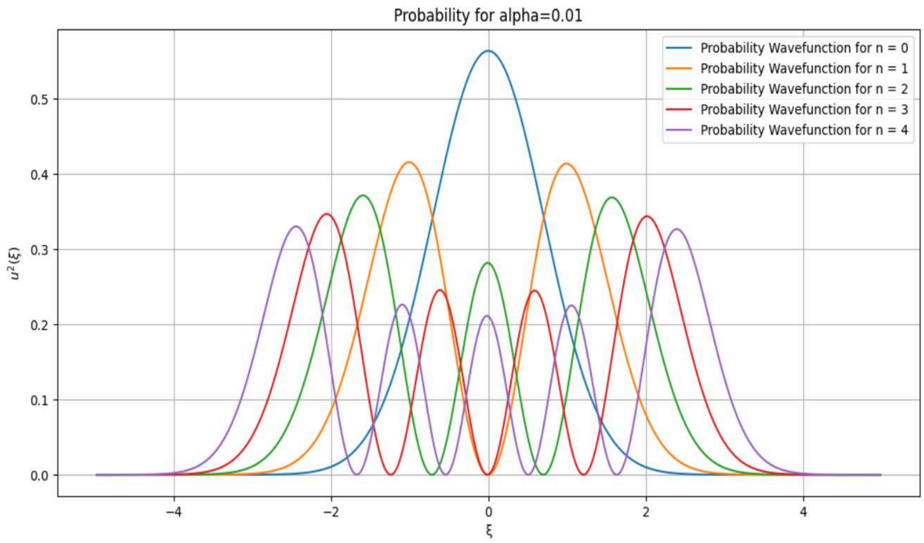

Figure 18:

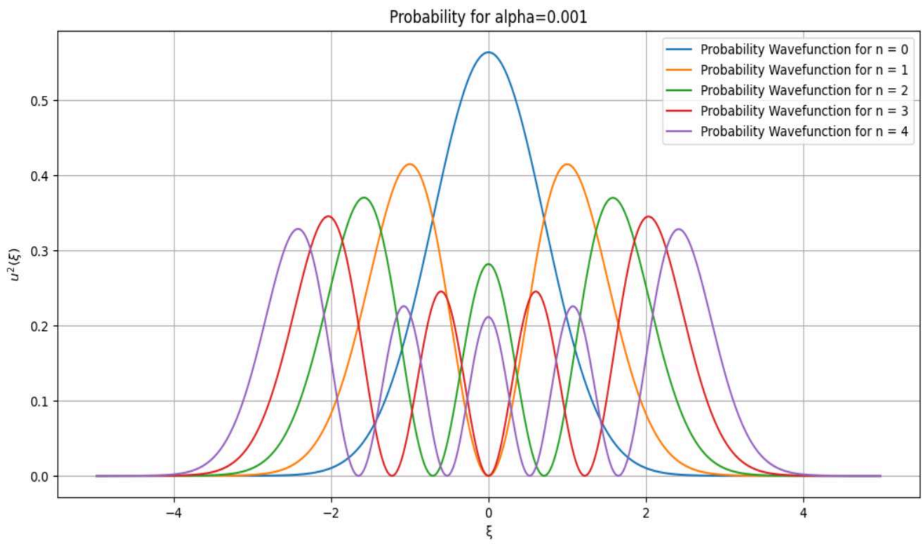

Figure 19:

5. Now these are the plots for the different value of **alpha** for the same state or same value of **n**.

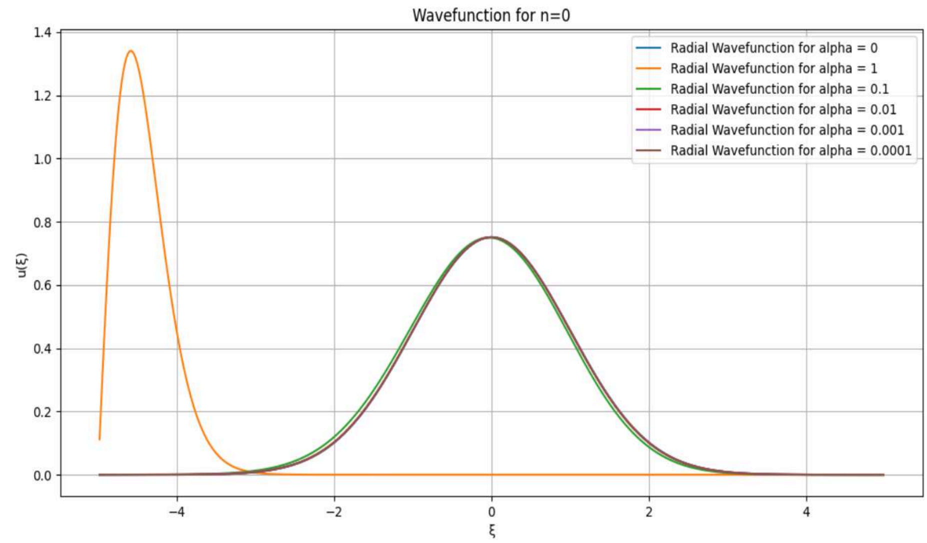

Figure 20:

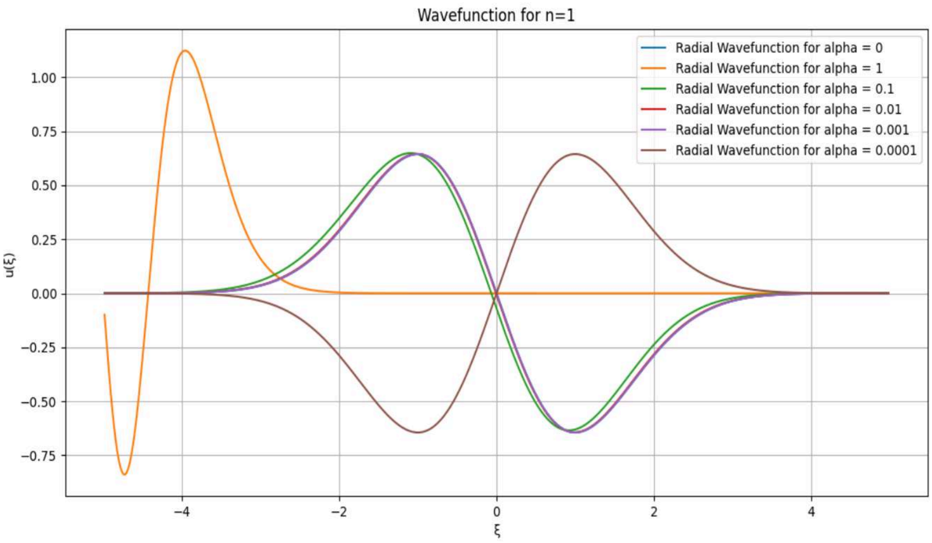

Figure 21:

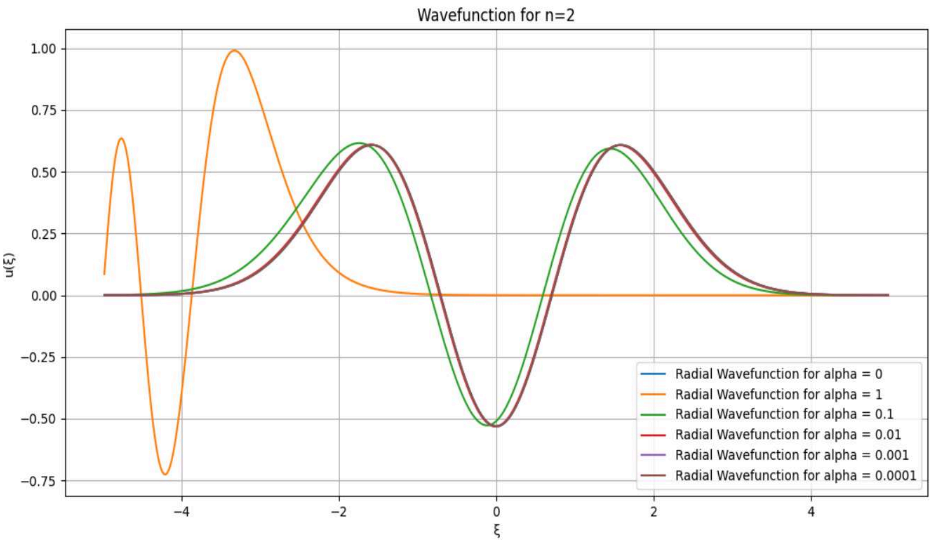

Figure 22:

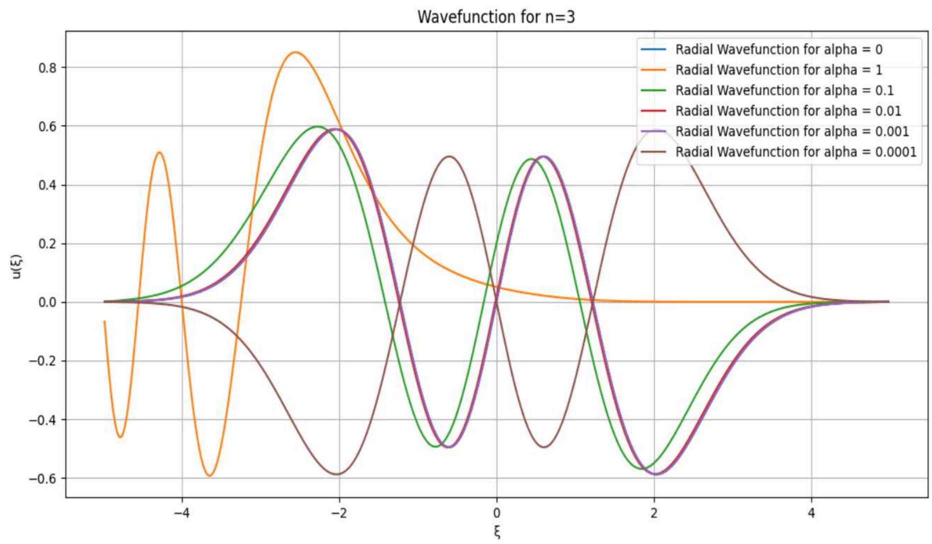

Figure 23:

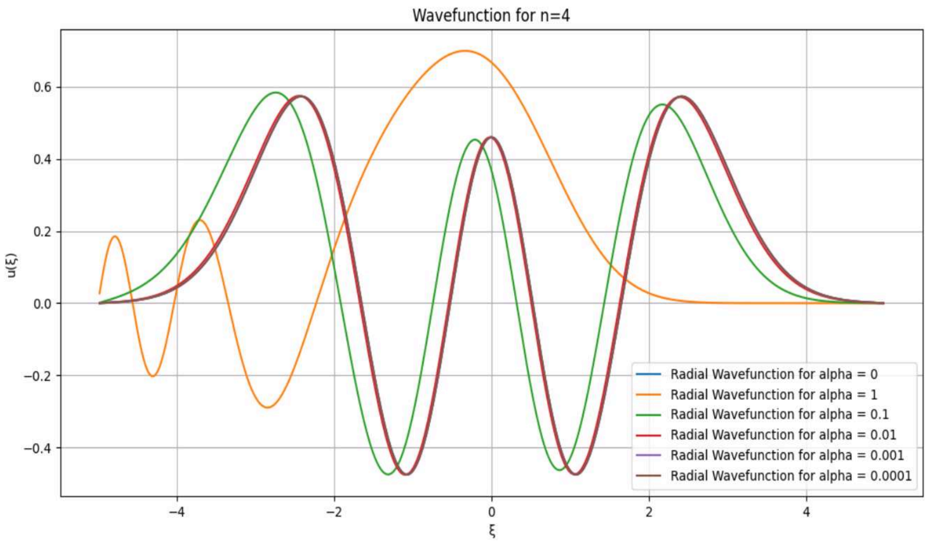

Figure 24:

6. The Probability Densities for above graphs are shown here.

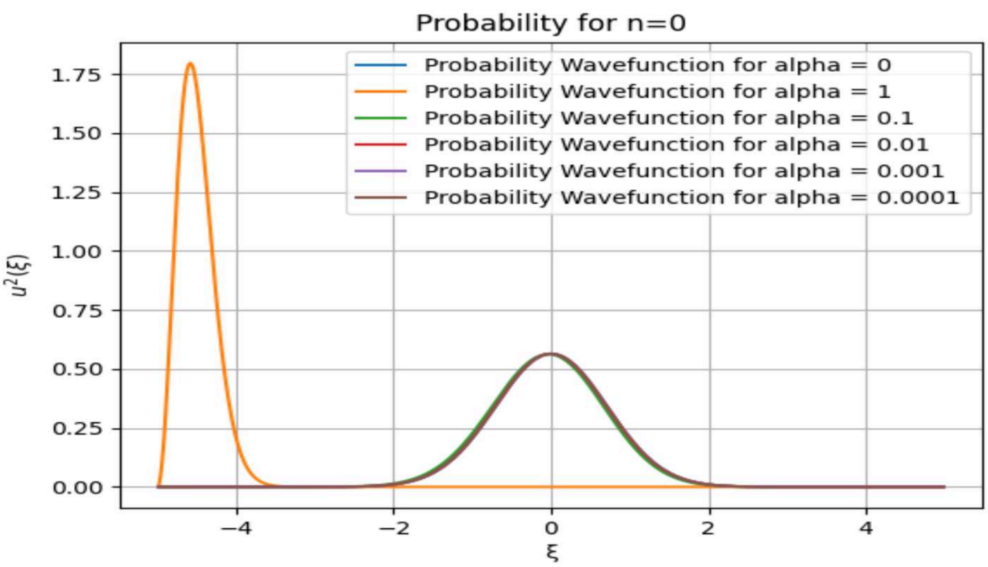

Figure 25:

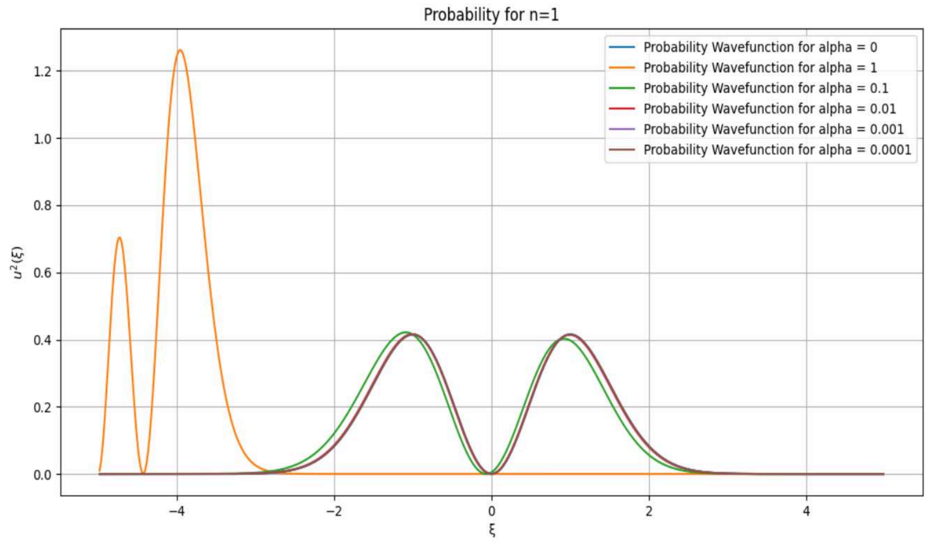

Figure 26:

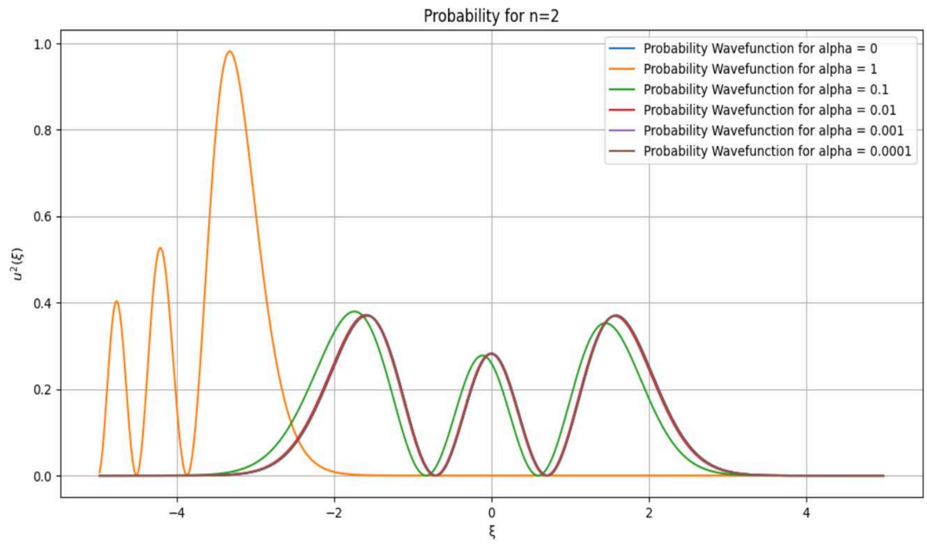

Figure 27:

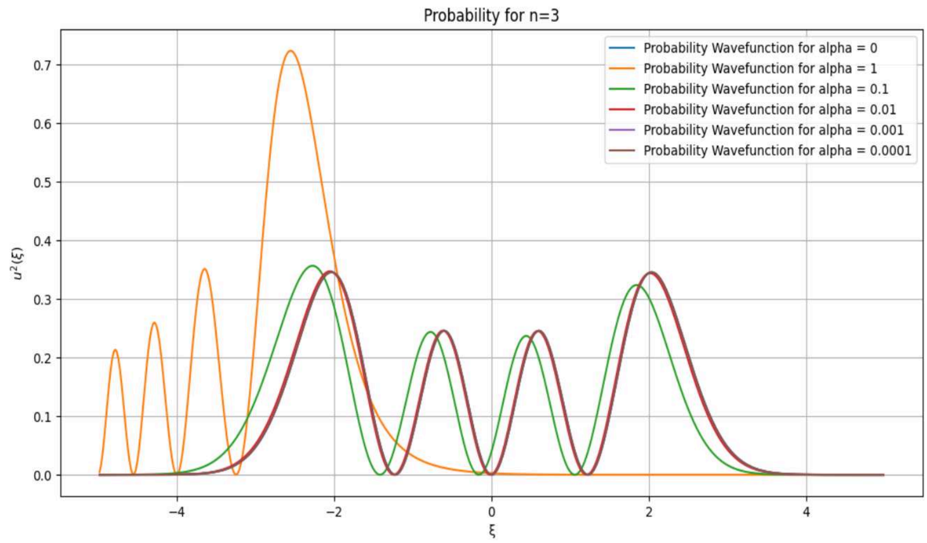

Figure 28:

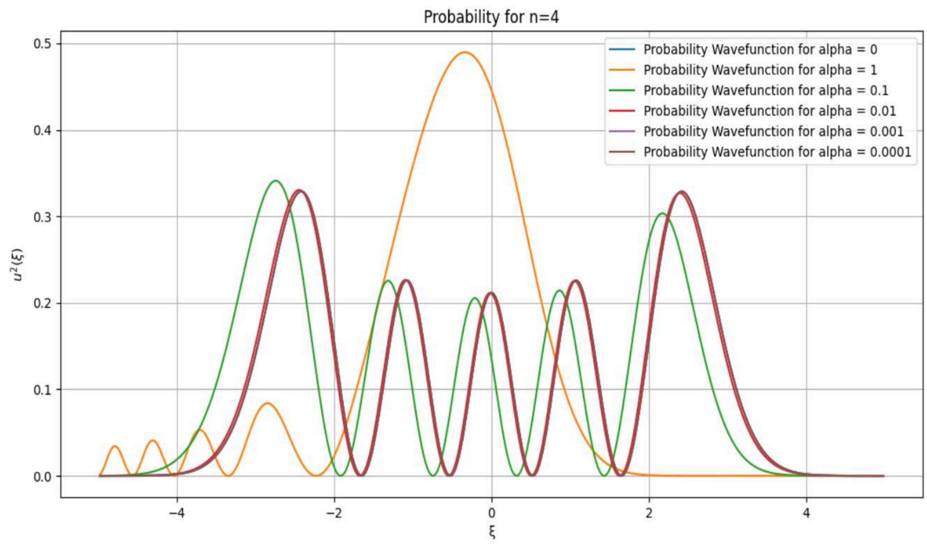

Figure 29:

7. In theory part we have to plot the potential for different values of **alpha**. So the plot is shown here

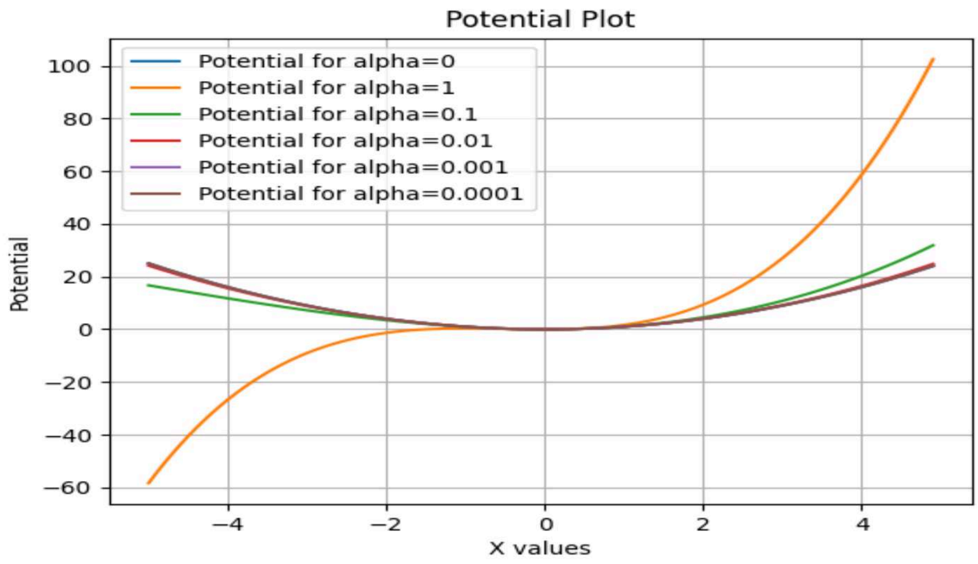

Figure 30:

B.Sc.(Hons.) Physics
32221501
Teacher: Mamta

S.G.T.B. Khalsa College
Quantum Mechanics (2022-23)
Lab Assignment # 13
Anharmonic Oscillator

Due Date and Time :
20.10.2022, 11:59PM
Max. Marks : 20

- The objective of this assignment is to estimate the eigenvalues and eigenvectors associated with the harmonic oscillator Hamiltonian perturbed with a cubic term.
- This assignment is based upon the problem 3 of the syllabus.

1. (6 marks) **Theory**
A particle of mass μ constrained to move in 1-dimension is subjected to the potential

$$V(x) = \frac{1}{2}kx^2 + bx^3\,; \quad k = \mu\,\omega^2. \tag{1}$$

   (a) Convert the equation into a dimensionless form by defining $x = \xi x_0$, where $x_0 = \sqrt{\hbar/\mu\,\omega}$ and ξ is the dimensionless position variable. Also define dimensionless potential energy $v(\xi) = V(x_0\,\xi)/E_0$ and dimensionless energy eigenvalue $\epsilon = E/E_0$ where $E_0 = \frac{1}{2}\hbar\omega$ is the ground state energy of the harmonic oscillator.
   (b) Plot the potential energy $v(\xi)$ as a function of ξ for $\alpha = 0$ and $\alpha = 10^{-q}$ with $q = 0$, 1, 2, 3, 4, where $\alpha = \frac{bx_0}{k}$.
   (c) Discuss what do you expect for the bound state eigen values.

2. (12 marks) **Programming**
   (a) Write a Python code to solve the Schrödinger Equation for a particle of mass $\mu = 940\,\mathrm{MeV/c^2}$ subjected to the potential given in equation (1) using any method known to you giving reasons for your choice of method. The code should
      i. obtain the first ten energy eigenvalues ϵ_n for each value of α mentioned above.
      ii. print the eigen values obtained along with the values given by second order perturbation theory[1] in a tabulated form rounded off to the first six significant digits.
      iii. plot ϵ_n as a function of n and compare the behaviour with that for harmonic oscillator.
   (b) Extend your program to print the energy eigenvalues in MeV.
   (c) Further extend your program to
      i. obtain the first five normalised eigenfunctions (dimensionless form) and corresponding probability densities in the range $[-\xi_{\max} : \xi_{\max}]$ with an appropriate value of $\xi_{\max}$.
      ii. plot these normalised wavefunctions for $\alpha = 0, 0.01, 0.1$ (all wavefunctions for one α in one plot). Verify that $\alpha = 0$ gives the same result as for harmonic oscillator.
      iii. plot the probability densities similarly.
      iv. plot the probability densities in ground state for $\alpha = 0$ and $\alpha = 10^{-q}$ with $q = 0, 1, 2, 3, 4$.
      v. Repeat above for the first excited state.

3. (2 marks) **Discussion**
Interpret and discuss your results.

---

[1] The perturbation theory estimates the energy eigenvalues upto second order to be (the reference will be shared with you along with the assignment):

$$\epsilon_n = (2n+1) - \frac{1}{8}\alpha^2\left[15(2n+1)^2 + 7\right]$$