Assignment 13 - Anharmonic Oscillator

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Theory:

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

$$\frac{d^2U}{dr^2} + \frac{2m}{\hbar^2}(E - V(r))U = 0$$

dimensionless

$$E = E_0 \, \mathcal{E}$$

↳ ground state

Let $x = r_0 \xi$ ⟶ dimensionless

r_0 ⟶ bohr radius

$$\frac{1}{r_0^2}\frac{d^2U}{d\xi^2} + \frac{2m}{\hbar^2}\left(E_0\mathcal{E} - \frac{1}{2}kr_0^2\xi^2 - \frac{1}{3}br_0^3\xi^3\right)U = 0$$

$$\frac{d^2U}{d\xi^2} + \frac{2mr_0^2}{\hbar^2}\left(E_0\mathcal{E} - \frac{1}{2}kr_0^2\xi^2 - \frac{1}{3}br_0^3\xi^3\right)U = 0$$

$$\frac{d^2U}{d\xi^2} + \left[\left(\frac{2mr_0^2E_0}{\hbar^2}\right)\mathcal{E} - \frac{2mr_0^4k}{2\hbar^2}\xi^2 - \frac{2mr_0^5\xi^3 b}{3\hbar^2}\right]U = 0$$

$$\frac{d^2U}{d\xi^2} + \left[\underbrace{\left(\frac{2mr_0^2E_0}{\hbar^2}\right)}_{\text{dimensionless}}\mathcal{E} - \underbrace{\frac{mkr_0^4}{\hbar^2}}_{\text{dimensionless}}(\xi^2) - \underbrace{\frac{2bmr_0^5}{3\hbar^2}}_{\text{dimensionless}}(\xi^3)\right]U = 0$$

$$\frac{2mr_0^2E_0}{\hbar^2} = 1 \qquad \frac{mkr_0^4}{\hbar^2} = 1$$

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

$$\frac{2m\left(\frac{\hbar^2}{mk}\right)^{1/2}E_0}{\hbar^2} = 1$$

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$$\frac{2m\hbar E_0}{(mk)^{1/2}} = \hbar^2$$

$$\frac{2m^{1/2} E_0}{k^{1/2}} = \hbar$$

$$E_0 = \frac{\hbar k^{1/2}}{2m^{1/2}} = \frac{\hbar}{2}\sqrt{\frac{k}{m}}$$

$$E_0 = \frac{\hbar\omega}{2}$$

→ $\frac{2bmr_0^5}{3\hbar^2}$ (third term)

$$\frac{2bm \cdot \hbar^2 \cdot r_0}{mk \cdot 3\hbar^2}$$

$$\boxed{\frac{2}{3}\frac{br_0}{k}}$$ → Let $\frac{br_0}{k} = \alpha$

$$\frac{d^2u}{d\xi^2} + \left[\varepsilon - \xi^2 - \frac{2}{3}\frac{br_0}{k}\xi^3\right]u = 0$$

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

dimensionless potential → $\boxed{\xi^2 + \frac{2}{3}\alpha\xi^3}$ → $V(\xi)$

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

$$= \left(n + \frac{1}{2}\right) 2$$

$$\boxed{\varepsilon = 2n + 1} \qquad n = 0, 1, 2 \ldots$$

(b)
(c)
} Done in Programming and Discussion

Programming

```
from scipy.linalg import eigh
import numpy as np
import matplotlib.pyplot as plt
from scipy.integrate import simps
import pandas as pd

def pot(x, alpha):
    return x**2 + (2/3)*alpha*x**3

def matrix_formation(a, b, N, f, alpha):

    x_range = np.linspace(a, b, N+1)
    h = x_range[1] - x_range[0]

    X = x_range[1: -1]

    l = np.zeros(len(X))
    d = np.zeros(len(X))
    u = np.zeros(len(X))
    potential = np.zeros(len(X))

    for i in range(0, len(X)):
        d[i] = -(-2/h**2)
        l[i] = -(1/h**2)
        u[i] = -(1/h**2)
        potential = f(X, alpha)

    diagonal = np.diag(d, k = 0)
    off_diag_l = np.diag(l[:-1], k = -1)
    off_diag_u = np.diag(u[:-1], k = 1)

    V = np.diag(potential, k = 0)

    matrix = diagonal + off_diag_l + off_diag_u + V

    return matrix, X

def perturbation(n, alpha):
    return 2*n + 1 - (1/8)*(alpha**2)*(15*(2*n+1)**2+7)

def normalize(x_vals, y_vals):
    norm = simps(abs(y_vals**2), x_vals)
    norm_result = y_vals/np.sqrt(norm)

    return x_vals, norm_result



x_values = np.linspace(-5, 5, 500)
alpha_vals = [0, 1e0, 1e-1, 1e-2, 1e-3, 1e-4]

for i in alpha_vals:
    plt.plot(x_values, pot(x_values, i), label = f'Alpha={i}')
plt.legend()
plt.grid()
plt.title(r'Potential Energy as a function of $\xi$')
plt.xlabel(r'\xi')
plt.ylabel(r'V(\xi)')
plt.show()


n_vals = np.array([0,1,2,3,4,5,6,7,8,9])


for i in alpha_vals:
```

```python

    matrix, X = matrix_formation(-5, 5, 500, pot, i)

    e , vec = eigh(matrix)

    perturbation_temp = perturbation(n_vals, i)

    data = {

  'n': n_vals,
  'Calculated eigen value': e[:10],
  'Perturbation eigen value': perturbation_temp,

    }

    df = pd.DataFrame(data)
    print(f'Alpha={i}')
    print('-----------------------------------------------------')
    print('Ground State Energy = ', 197.3/2*np.sqrt(100/940)*e[0], 'MeV')
    print(df)

    plt.plot(n_vals , e[:10], label = f'alpha={i}')

plt.legend()
plt.grid()
plt.title(r'E(n) as a function of n')
plt.xlabel(r'E(n)')
plt.ylabel(r'n')
plt.show()


for i in alpha_vals:

    for j in range(0,5):

        matrix, X = matrix_formation(-5, 5, 500, pot, i)

        e , vec = eigh(matrix)

        plt.plot(X, normalize(X, vec.T[j])[1], label = f'n = {j}')
    plt.legend()
    plt.grid()
    plt.title(f'Wave Function Alpha={i}')
    plt.xlabel(r'\xi')
    plt.ylabel(r'U(\xi)')
    plt.show()

for i in alpha_vals:

    for j in range(0,5):

        matrix, X = matrix_formation(-5, 5, 500, pot, i)

        e , vec = eigh(matrix)

        plt.plot(X, (normalize(X, vec.T[j])[1])**2, label = f'n = {j}')
    plt.legend()
    plt.grid()
    plt.title(f'Probability Density Alpha={i}')
    plt.xlabel(r'\xi')
    plt.ylabel(r'U(\xi)')
    plt.show()


for i in range(0,2):

    for j in alpha_vals:
```

```

        matrix , X = matrix_formation(-5, 5, 500, pot , j)

        e , vec = eigh(matrix)

        plt.plot(X, normalize(X, vec.T[i])[1], label = f'alpha = {j}')
    plt.legend()
    plt.grid()
    plt.title(f'Wave Function n={i}')
    plt.xlabel(r'\xi')
    plt.ylabel(r'U(\xi)')
    plt.show()

for i in range(0,2):

    for j in alpha_vals:

        matrix , X = matrix_formation(-5, 5, 500, pot , j)

        e , vec = eigh(matrix)

        plt.plot(X, (normalize(X, vec.T[i])[1])**2, label = f'alpha = {j}')
    plt.legend()
    plt.grid()
    plt.title(f'Probability Density n={i}')
    plt.xlabel(r'\xi')
    plt.ylabel(r'U(\xi)')
    plt.show()
```

Result and Discussion

I chose the Finite difference Method as it is the most efficient and accurate.

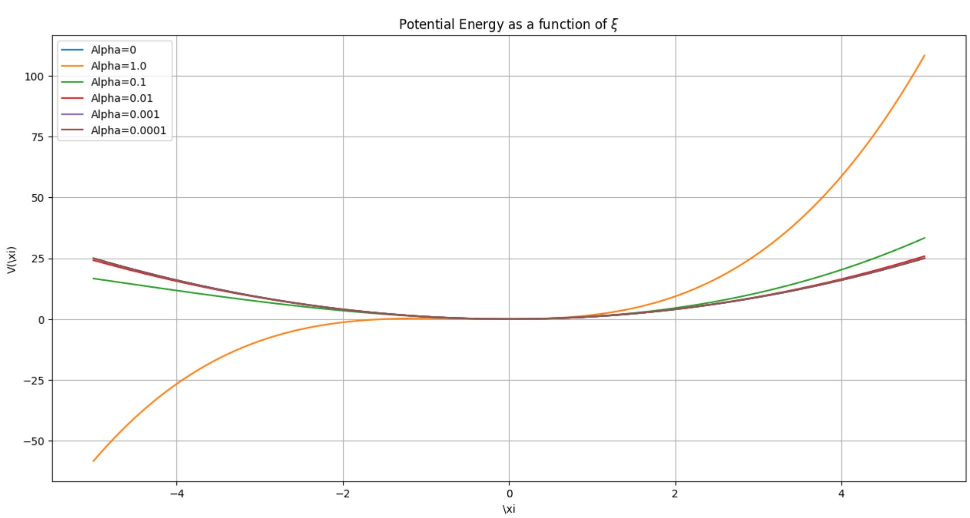

Figure 1: Potential as a function of ξ

Graph of the potential as a function of ξ for different values of alpha.

Alpha=0

Ground State Energy = 32.17527778616816 MeV

	n	Calculated eigen value	Perturbation eigen value
0	0	0.999975	1.0
1	1	2.999875	3.0
2	2	4.999675	5.0
3	3	6.999377	7.0
4	4	8.999000	9.0
5	5	10.998672	11.0
6	6	12.999078	13.0
7	7	15.003019	15.0
8	8	17.019260	17.0
9	9	19.068417	19.0

Figure 2: Alpha=0

Alpha=1.0

Ground State Energy = -1072.5444847161077 MeV

	n	Calculated eigen value	Perturbation eigen value
0	0	-33.333595	-1.75
1	1	-17.954430	-14.75
2	2	-7.870886	-42.75
3	3	-1.399264	-85.75
4	4	0.864462	-143.75
5	5	2.454161	-216.75
6	6	4.582061	-304.75
7	7	7.061949	-407.75
8	8	9.798874	-525.75
9	9	12.758779	-658.75

Figure 3: Alpha=1

Alpha=0.1

Ground State Energy = 32.07578690408526 MeV

	n	Calculated eigen value	Perturbation eigen value
0	0	0.996883	0.9725
1	1	2.979703	2.8225
2	2	4.944703	4.5225
3	3	6.891146	6.0725
4	4	8.818697	7.4725
5	5	10.730017	8.7225
6	6	12.639217	9.8225
7	7	14.582078	10.7725
8	8	16.606189	11.5725
9	9	18.743220	12.2225

Figure 4: Alpha=0.1

Alpha=0.01

Ground State Energy = 32.17429458883316 MeV

	n	Calculated eigen value	Perturbation eigen value
0	0	0.999944	0.999725
1	1	2.999678	2.998225
2	2	4.999145	4.995225
3	3	6.998347	6.990725
4	4	8.997304	8.984725
5	5	10.996156	10.977225
6	6	12.995638	12.968225
7	7	14.998739	14.957725
8	8	17.014655	16.945725
9	9	19.064520	18.932225

Figure 5: Alpha=0.01

```
Alpha=0.001
------------------------------------------------------
Ground State Energy =  32.17526795533855 MeV
   n  Calculated eigen value  Perturbation eigen value
0  0                0.999975                  0.999997
1  1                2.999873                  2.999982
2  2                4.999670                  4.999952
3  3                6.999367                  6.999907
4  4                8.998983                  8.999847
5  5               10.998647                 10.999772
6  6               12.999043                 12.999682
7  7               15.002976                 14.999577
8  8               17.019214                 16.999457
9  9               19.068378                 18.999322
```

Figure 6: Alpha=0.001

```
Alpha=0.0001
------------------------------------------------------
Ground State Energy =  32.17527768786347 MeV
   n  Calculated eigen value  Perturbation eigen value
0  0                0.999975                  1.000000
1  1                2.999875                  3.000000
2  2                4.999675                  5.000000
3  3                6.999377                  6.999999
4  4                8.999000                  8.999998
5  5               10.998672                 10.999998
6  6               12.999077                 12.999997
7  7               15.003018                 14.999996
8  8               17.019260                 16.999995
9  9               19.068417                 18.999993
```

Figure 7: Alpha=0.0001

The comparison of calculated values with the perturbation eigne values.

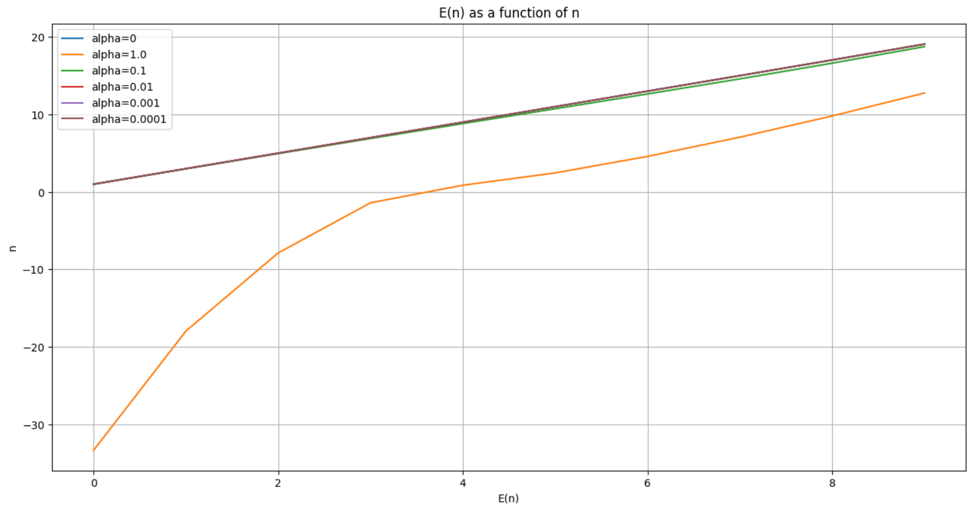

Figure 8: Energy eigen values as a function of n

Graph for E(n) as a function of n.

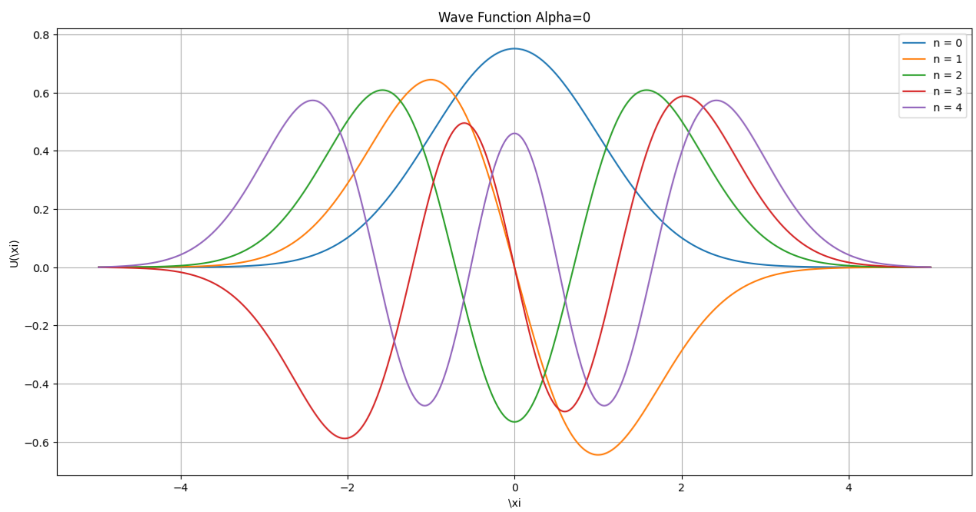

Figure 9: First Five Wave Functions

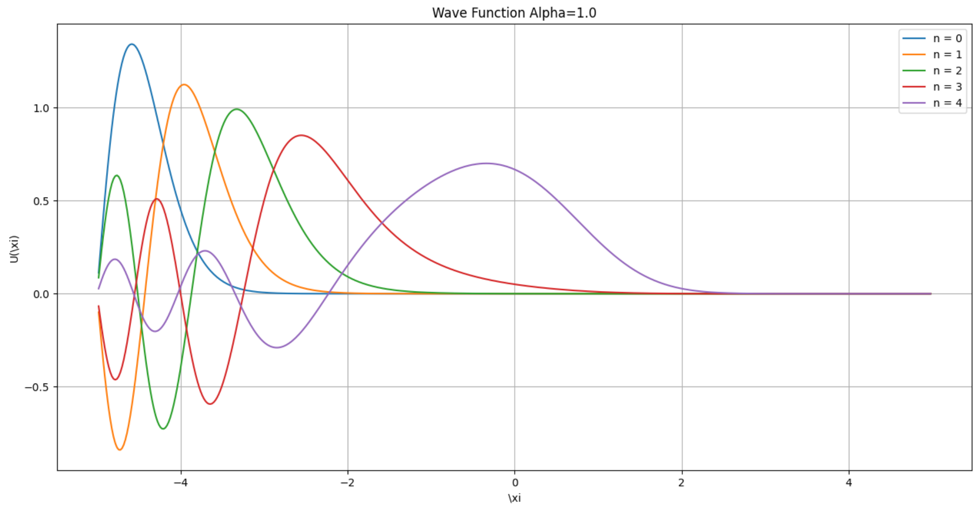

Figure 10: First Five Wave Functions

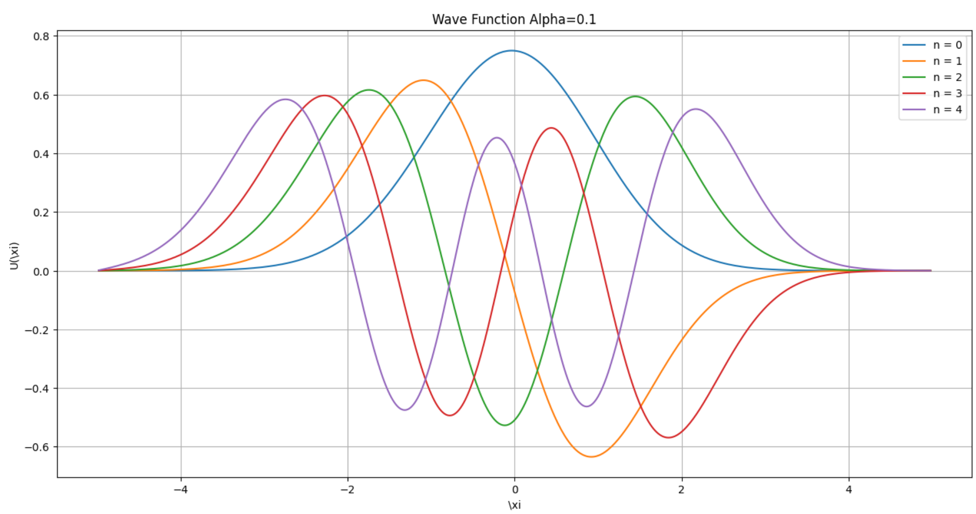

Figure 11: First Five Wave Functions

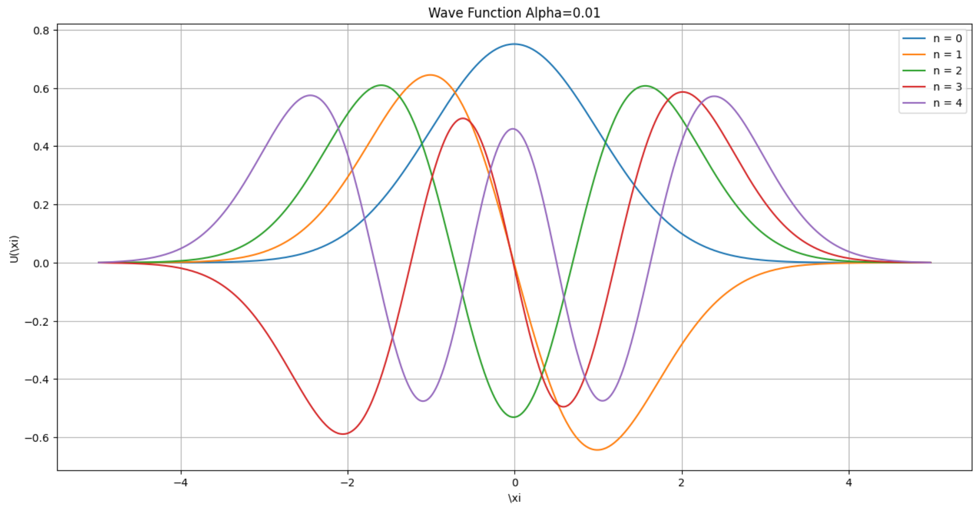

Figure 12: First Five Wave Functions

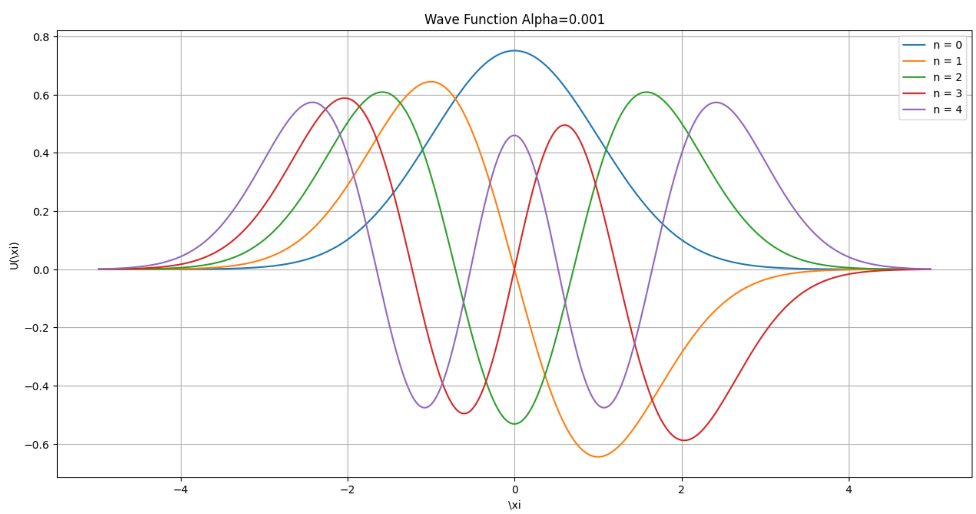

Figure 13: First Five Wave Functions

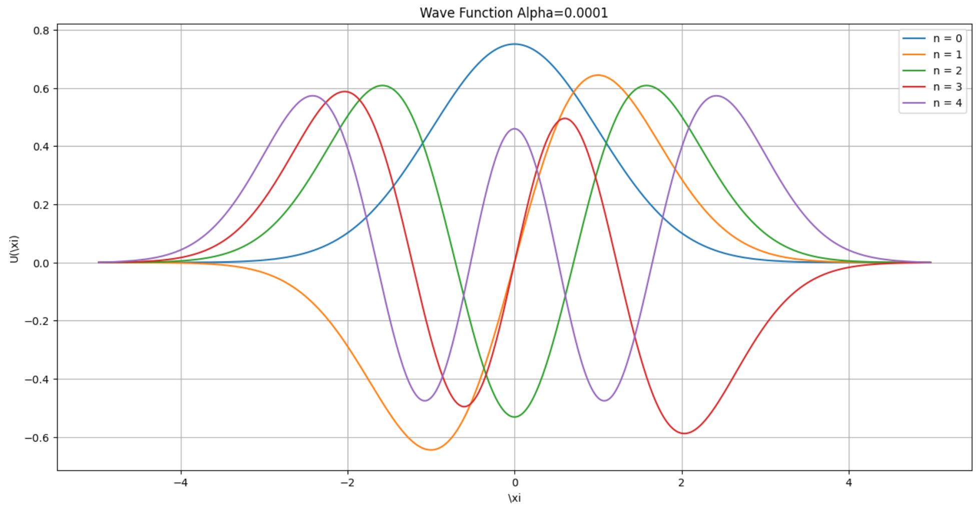

Figure 14: First Five Wave Functions

First Five Wave Functions for each value of alpha.

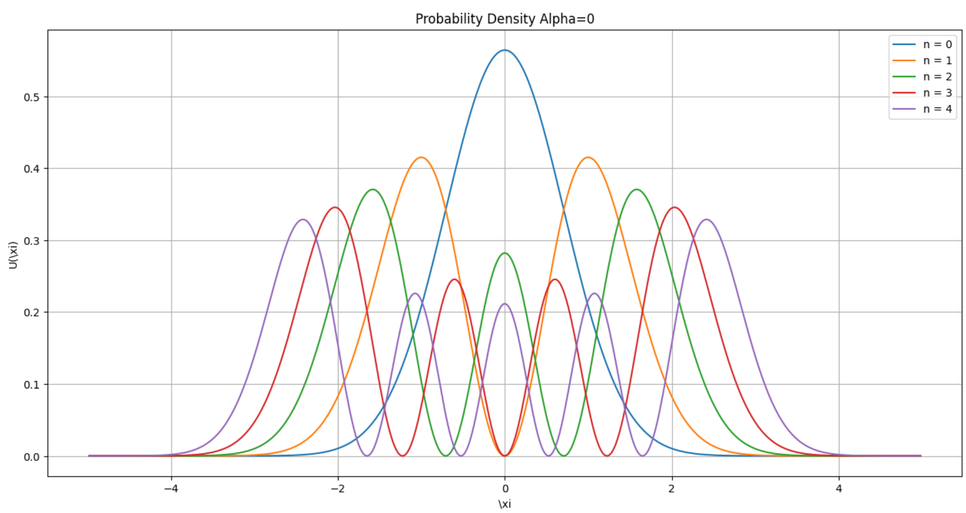

Figure 15: First Five Probability Densities

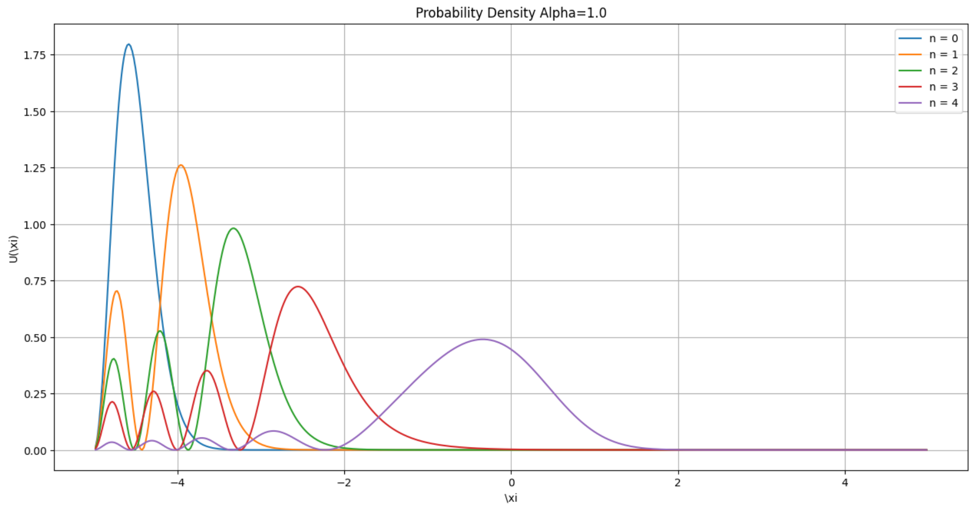

Figure 16: First Five Probability Densities

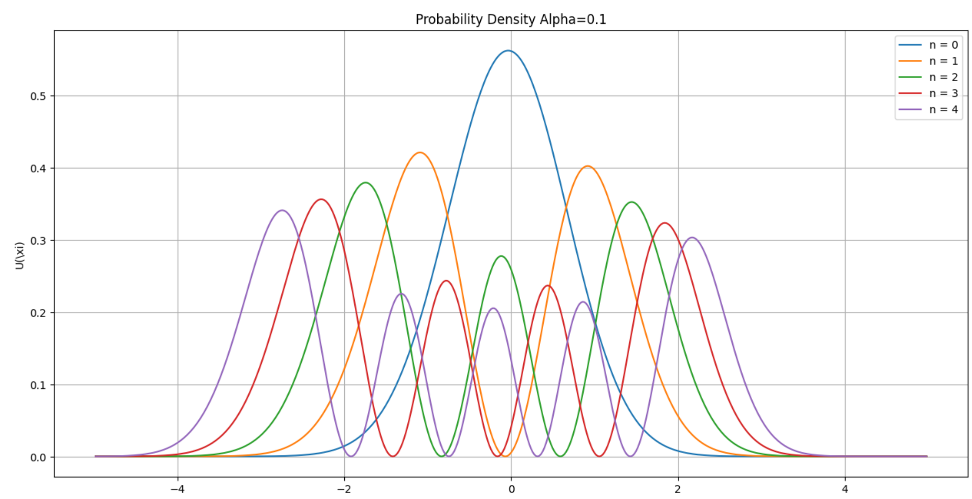

Figure 17: First Five Probability Densities

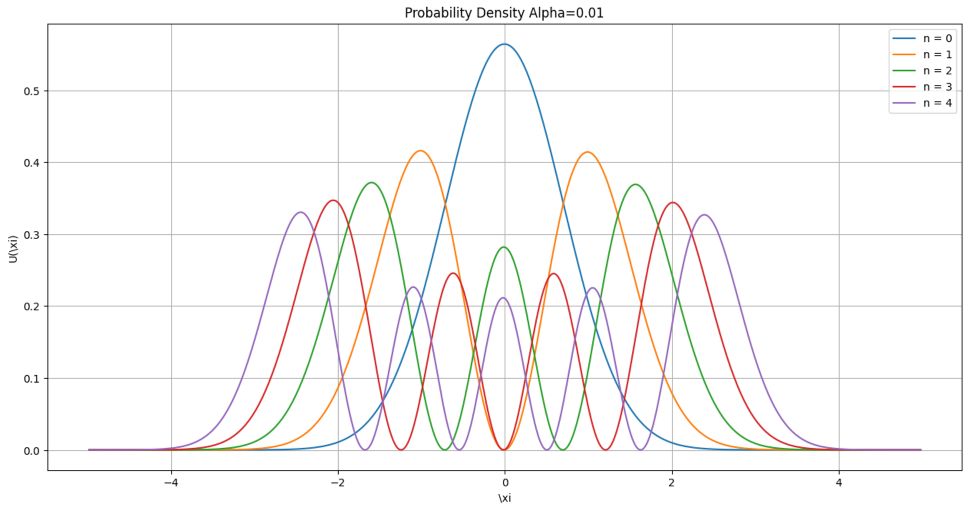

Figure 18: First Five Probability Densities

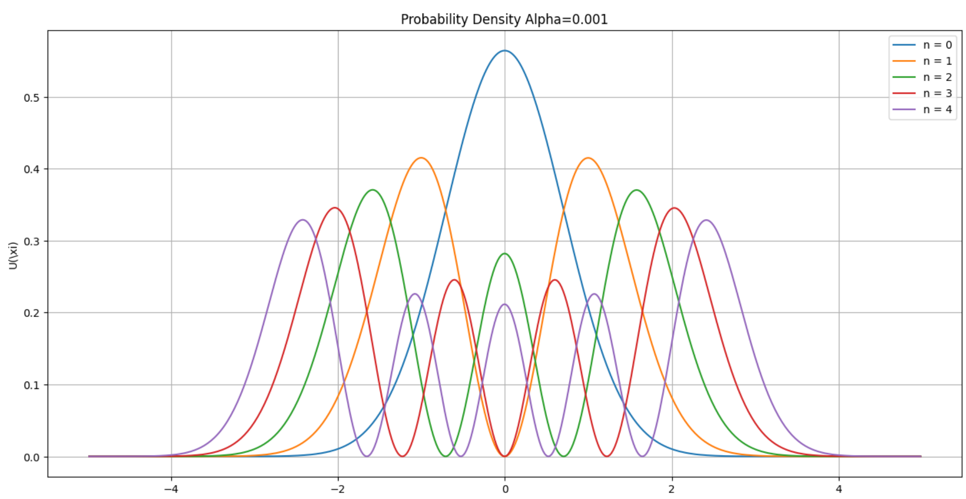

Figure 19: First Five Probability Densities

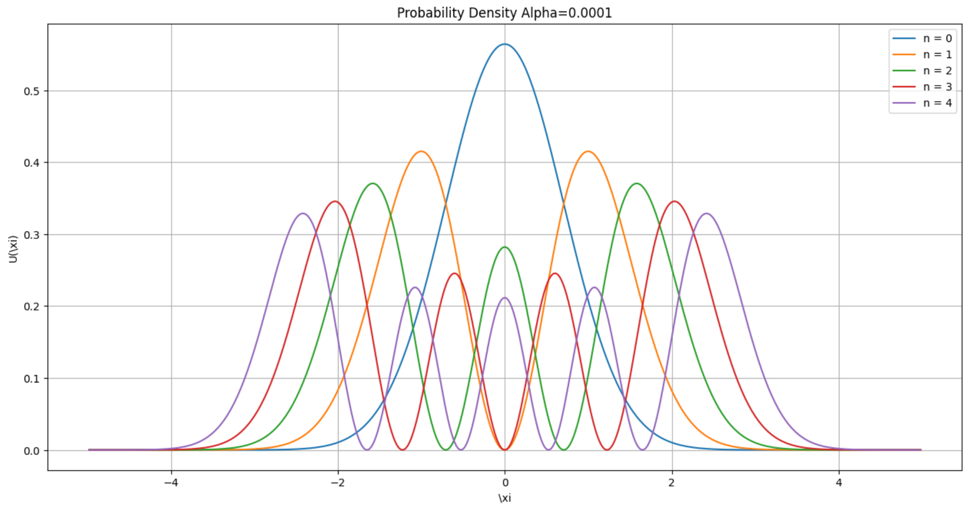

Figure 20: First Five Probability Densities

First Five Probability Densities for each value of alpha.

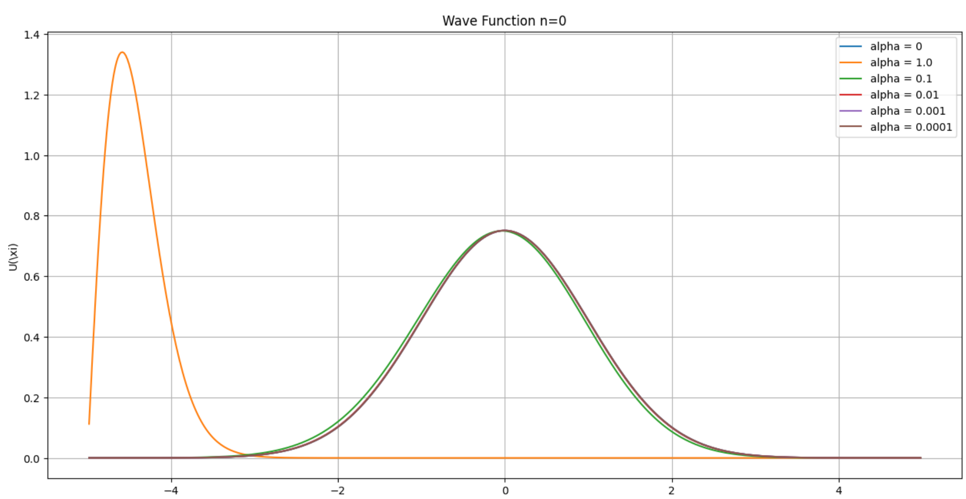

Figure 21: Ground State

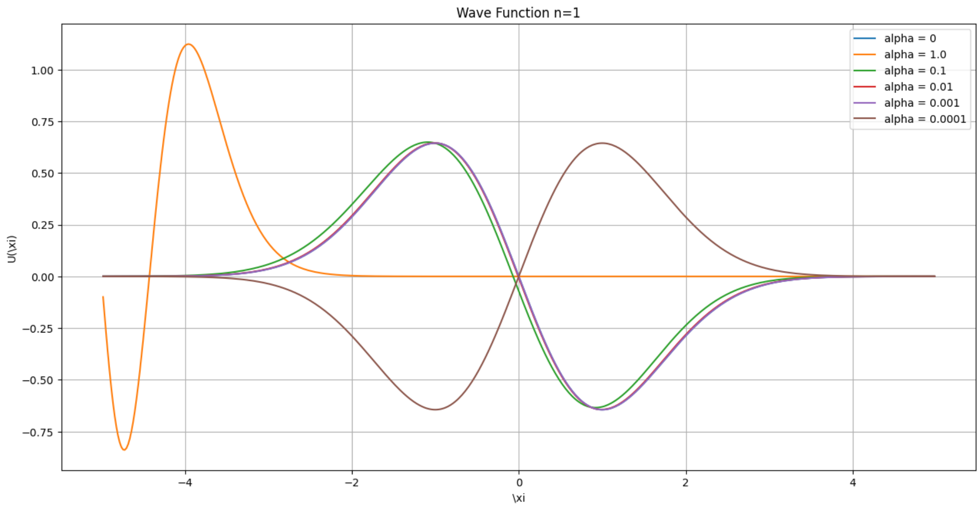

Figure 22: First Excited State

Ground State and Excited State variation with alpha.

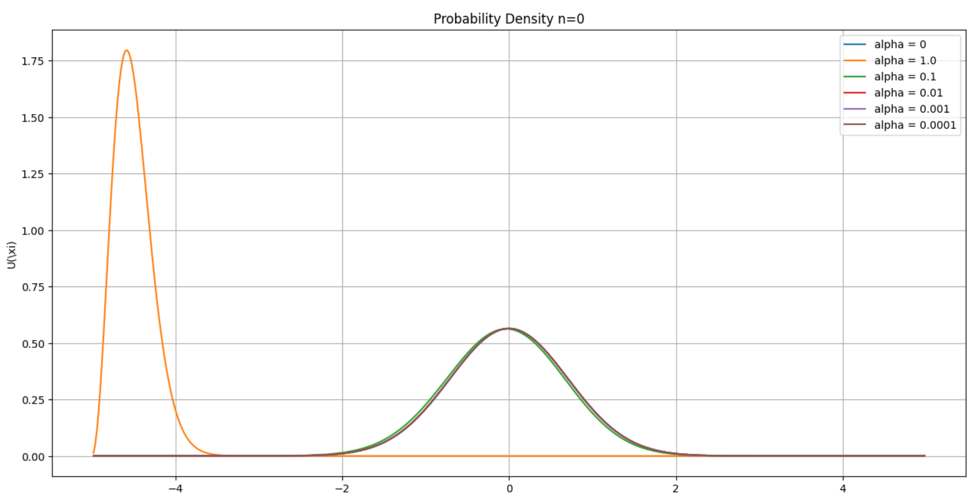

Figure 23: Ground State Probability

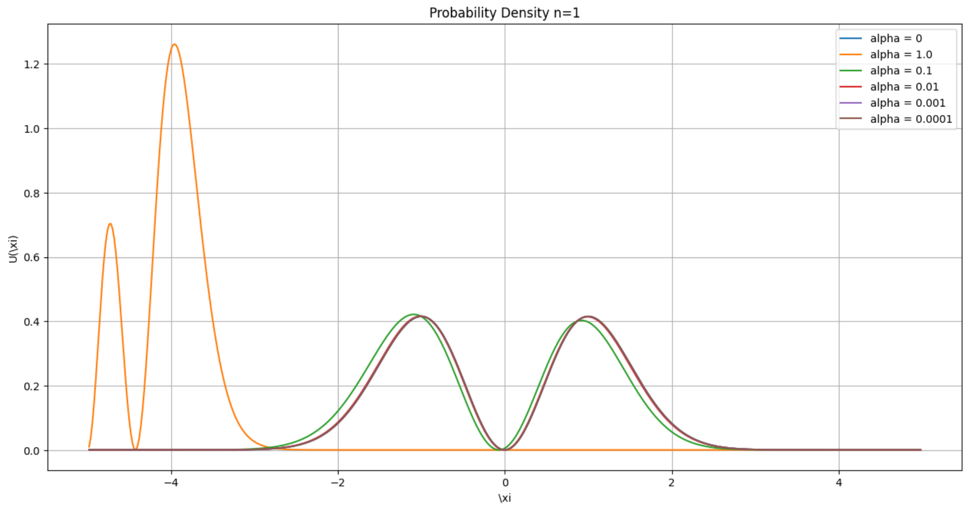

Figure 24: First Excited State Probability

Ground State probability and First Excited State probability variation with alpha.

Some notable observations from all the figures are:

- As the value of alpha decreases and approaches 0 the solution approaches the harmonic oscillator.
- The values and graphs for alpha=1 are very different from the rest, this is due to the fact that when alpha=1 or is large then the x^3 term dominates the potential function and hence the results are different.