Assignment 13 - Anharmonic Oscillator

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Assignment 13 (Anharmonic Oscillator)

Date ..../..../.........

The given potential is:

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

(a)

TISE is

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

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

To make r and E dimensionless

Take

$$r = r_0\xi_1 \qquad \& \quad \varepsilon = \varepsilon_0 E$$

Now,
$$\frac{du}{dr} = \frac{du}{d\xi_1}\left(\frac{d\xi}{dr}\right)$$

$$\frac{du}{dr} = \frac{1}{r_0}\frac{du}{d\xi_1}$$

Again differentiating w.r.t. r

$$\frac{d^2u}{dr^2} = \frac{1}{r_0^2}\frac{d^2u}{d\xi_1^2}$$

Putting above $\frac{d^2u}{d\xi_1^2}$ in (1)

$$\frac{d^2u}{d\xi_1^2} + \frac{2mr_0^2}{\hbar^2}\left[\varepsilon_0 E - \frac{1}{2}k(r_0\xi_1)^2 - \frac{1}{3}b(r_0\xi_1)^3\right]u = 0$$

$$\frac{d^2u}{d\xi_1^2} + \frac{2m}{\hbar^2}\left[\varepsilon_0 E r_0^2 - \frac{1}{2}kr_0^4\xi_1^2 - \frac{1}{2}br_0^5\xi_1^3\right]u = 0$$

$$\frac{d^2u}{d\xi_1^2} + \left[\frac{2m\varepsilon_0 r_0^2}{\hbar^2}E - \frac{mkr_0^4}{\hbar^2}\xi_1^2 - \frac{2mbr_0^5\xi_1^3}{3\hbar^2}\right]u = 0 \quad -(2)$$

To find these in dimensionless form, we'll equate coefficients of ξ_1^2, E & ξ_1^5 equals to 1 one by one.

Spiral

Date ..../..../.........

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

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

$$\frac{2m b_0^2 \mathcal{E}_0}{\hbar^2} = 1$$

$$\mathcal{E}_0 = \frac{\hbar^2}{2m r_0^2} = \frac{\hbar^2}{2m}\frac{(mk)^{1/2}}{(\hbar^2)^{1/2}} = \frac{\hbar}{2m}(mk)^{1/2}$$

$$\mathcal{E}_0 = \frac{\hbar}{2}\sqrt{\frac{k}{m}} = \frac{\hbar\omega}{2}$$

Now, for coefficients of ε_1^5

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

$$\frac{2mb}{3\hbar^2}\left(\frac{\hbar^2}{mk}\right)^{5/4} = \frac{2mb}{mk} \times \frac{\hbar^2}{3\hbar^2} r_0 = \frac{2}{3}\frac{br_0}{k}$$

Now take

$$\frac{br_0}{k} = \alpha$$

putting all of these in Eq^n (2)

$$\frac{d^2u}{d\varepsilon_1^2} + \left[\varepsilon - \varepsilon_1^2 - \frac{2}{3}\frac{br_0}{k}\varepsilon_1^3\right]u = 0$$

$$\frac{d^2u}{d\varepsilon_1^2} + \left[\varepsilon - \left(\varepsilon_1^2 + \frac{2}{3}\alpha\varepsilon_1^3\right)\right]u = 0$$

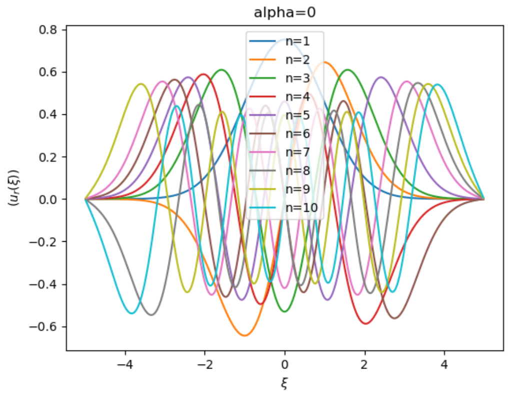
Dimensionless potential becomes $\rightarrow$ $\left[\varepsilon_1^2 + \frac{2}{3}\alpha\varepsilon_1^3\right] \rightarrow V(\varepsilon_1)$

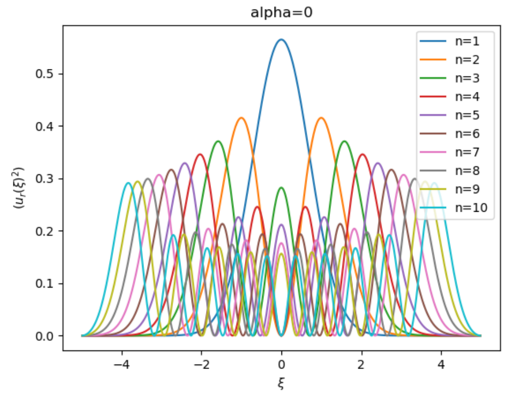
For defining ε

$$\varepsilon = \frac{\mathcal{E}}{\mathcal{E}_0} = \frac{(n+\frac{1}{2})\hbar\omega}{\frac{\hbar\omega}{2}} = 2n+1$$

Programming

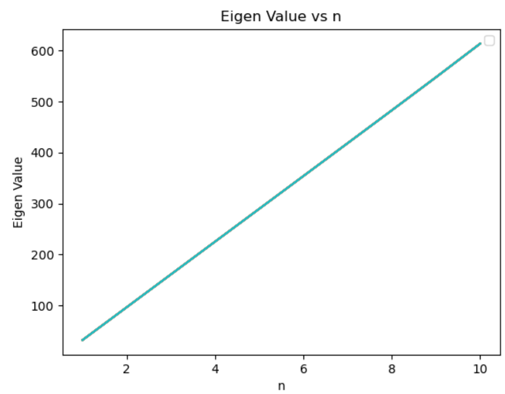
```python
import numpy as np
from scipy.linalg import eigh
import matplotlib.pyplot as plt
import scipy.integrate as integrate
import pandas as pd
from scipy.special import assoc_laguerre
from scipy.optimize import fsolve
def diag_mat(xi,xf,N,l):
    X = np.linspace(xi,xf,N+2)
    x=X[1:-1]
    h = x[1]-x[0]
    a,v=np.zeros((len(x),len(x))),np.zeros((len(x),len(x)))
    for i in range(len(x)):
        for j in range(len(x)):
            if i==j:
                a[i][i]=2/h**2
                v[i][i]= ((x[i]**2)) +((2/3)*(const)*(x[i]**3))
            elif i==j+1:
                a[i][j]=-1/h**2
            elif i == j-1:
                a[i][j] = -1/h**2
    A=(a+v)
    eig = eigh(A)
    return eig,x

def graph(x,y,label,xlabel,ylabel,title):
    plt.plot(x,y,label=label)
    plt.xlabel(xlabel)
    plt.ylabel(ylabel)
    plt.title(title)
    plt.grid()
    plt.legend()

N=500;const_=[0];no_eigen_values=10;conversion_factor=(197.3/2)*np.sqrt(100/940)
for i in range(0,4,1):
    const_.append(10**-i)
k=100;m=940;h_cut=6.5821*(10**-22);r0=np.power((h_cut**2)/m*k,1/4)
for const in const_:
    U_a=[];anal_eig_val=[];state=[]
    for i in range(0,no_eigen_values,1):
        state.append(i+1)
        anal_eig_val.append(((2*i+1)-(1/8)*((const)**2)*(15*np.power((2*i+1),2)+7))*conversion_factor)
        xi=-5;xf=5
        U_,x=diag_mat(xi,xf,N,0)
        U=U_[1][:,i]
        U_a=(U_[0][:no_eigen_values])*conversion_factor
        u_norm=U/np.sqrt(integrate.simps(np.power(U,2),x))
        # graph(x,np.power(u_norm,1),f'n={i+1}',"$\u03BE$","$(u_r(\u03BE))$",f'alpha={const}')
        # graph(x,np.power(u_norm,2),f'n={i+1}',"$\u03BE$","$(u_r(\u03BE)^2)$",f'alpha={const}')
        graph(np.arange(1,no_eigen_values+1,1),U_a,None,"n","Eigen Value","Eigen Value vs n")
    plt.show()

#---------------------Q-a(ii)-------------------------#
    print("Eigen Values for different alpha=",const)
    data ={
        "n":state,
        "Numerical Eigen Values ": U_a,
        "Analytical Eigen Values ":anal_eig_val ,
    }
    print(pd.DataFrame(data))
```



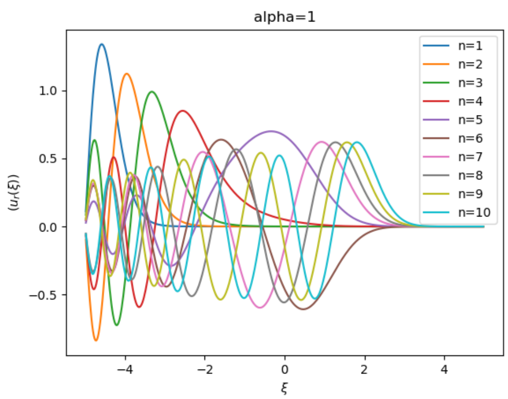


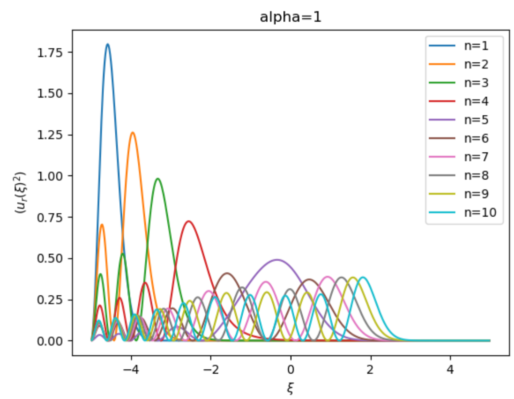
Eigen Values for different alpha= 0

	n	Numerical Eigen Values	Analytical Eigen Values
0	1	32.175281	32.176082
1	2	96.524241	96.528247
2	3	160.870000	160.880411
3	4	225.212622	225.232575
4	5	289.552700	289.584740
5	6	353.894373	353.936904
6	7	418.259665	418.289069
7	8	482.738729	482.641233
8	9	547.613596	546.993397
9	10	613.547575	611.345562



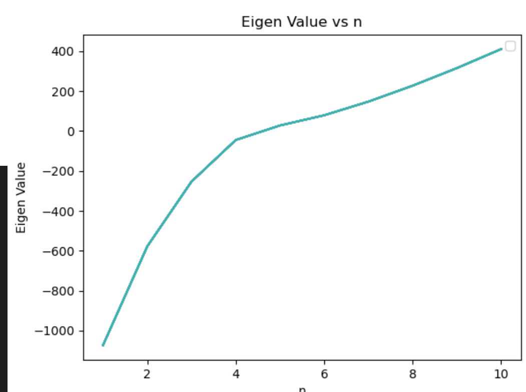
Result and Discussion

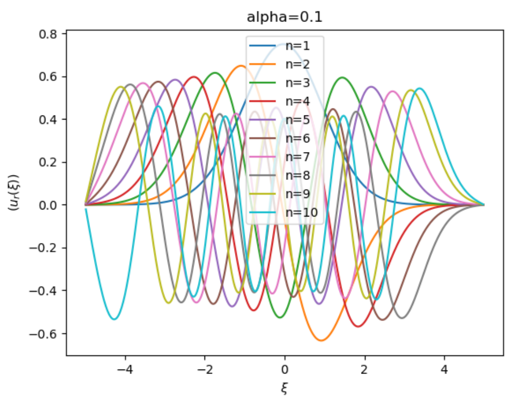


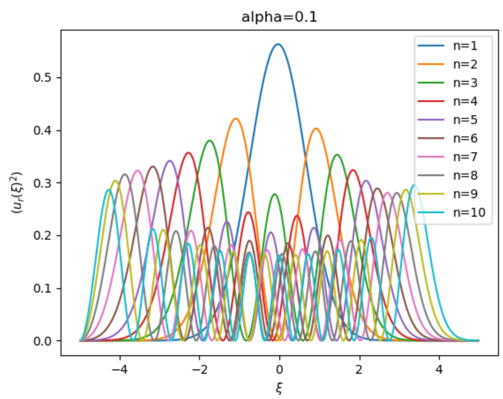


Eigen Values for different alpha= 1

	n	Numerical Eigen Values	Analytical Eigen Values
0	1	-1072.544034	-56.308144
1	2	-577.702207	-474.597212
2	3	-253.253015	-1375.527514
3	4	-45.021813	-2759.099049
4	5	27.815192	-4625.311817
5	6	78.965863	-6974.165818
6	7	147.433537	-9805.661051
7	8	227.226851	-13119.797518
8	9	315.290667	-16916.575218
9	10	410.529169	-21195.994151

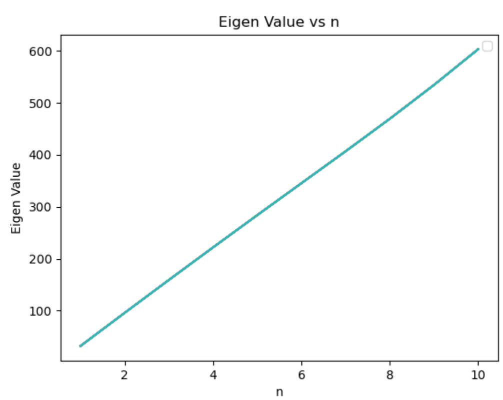


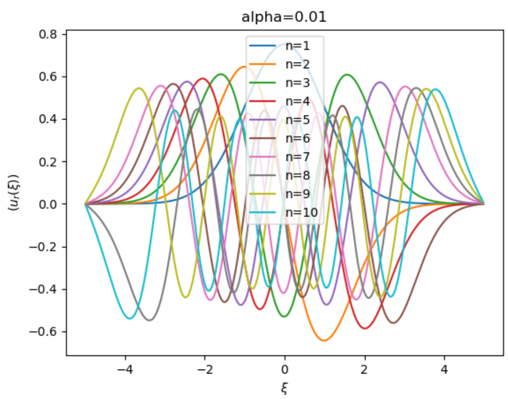


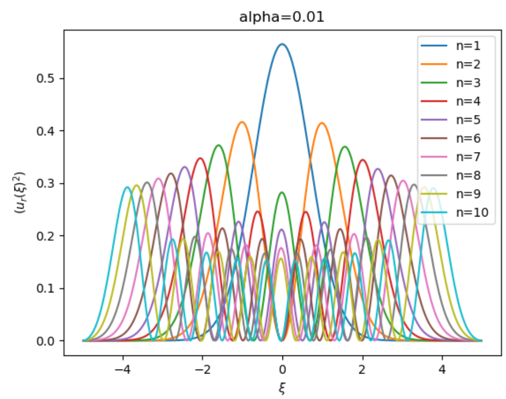


Eigen Values for different alpha= 0.1

	n	Numerical Eigen Values	Analytical Eigen Values
0	1	32.075790	31.291240
1	2	95.875183	90.816992
2	3	159.101208	145.516332
3	4	221.730145	195.389259
4	5	283.751247	240.435774
5	6	345.250097	280.655877
6	7	406.680726	316.049567
7	8	469.194478	346.616846
8	9	534.322584	372.357711
9	10	603.084011	393.272165

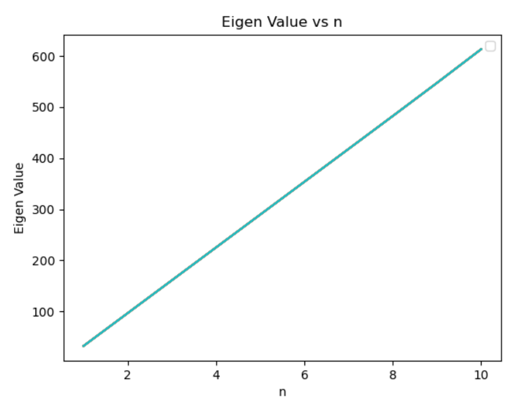


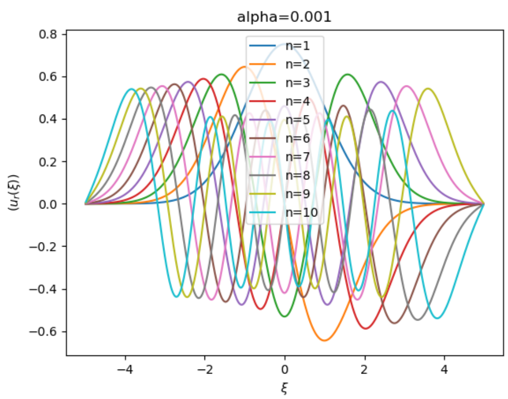


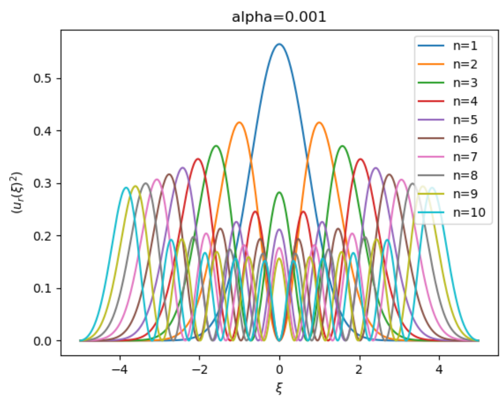


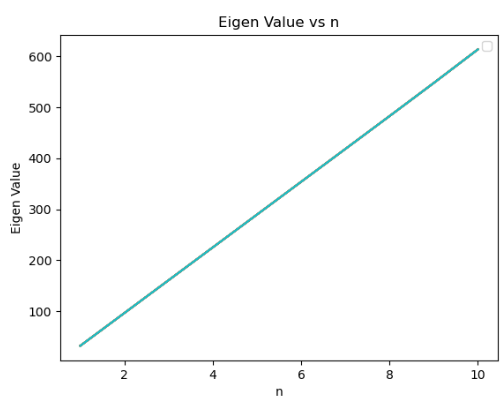
Eigen Values for different alpha= 0.01

	n	Numerical Eigen Values	Analytical Eigen Values
0	1	32.174298	32.167234
1	2	96.517894	96.471134
2	3	160.852927	160.726770
3	4	225.179463	224.934142
4	5	289.498140	289.093250
5	6	353.813421	353.204094
6	7	418.148996	417.266674
7	8	482.601010	481.280989
8	9	547.465423	545.247041
9	10	613.422185	609.164828









Eigen Values for different alpha= 0.001

	n	Numerical Eigen Values	Analytical Eigen Values
0	1	32.175271	32.175994
1	2	96.524177	96.527675
2	3	160.869830	160.878875
3	4	225.212291	225.229591
4	5	289.552155	289.579825
6	7	418.258559	418.278845
7	8	482.737351	482.627631
8	9	547.612113	546.975934
9	10	613.546318	611.323755