NAME: ANURAG DAS

ROLL No.: 2020PHY1116

QUANTUM MECHANICS
(LAB)

SEMESTER - V

ASSIGNMENT-13

Ans (a) $-\frac{\hbar^2}{2m}\frac{d^2u}{dx^2} + V(x)\,u = E\,u$

$$\frac{d^2u}{dx^2} + \frac{2m}{\hbar^2}(E-V)\,u = 0 \qquad \text{--- (1)}$$

Put $x = x_0\xi$, $\boxed{E = \epsilon_0 \mathcal{E}}$

$$\frac{du}{dx} = \frac{du}{d\xi}\frac{d\xi}{dx}$$

$$\boxed{\frac{du}{dx} = \frac{1}{x_0}\frac{du}{d\xi}}$$

$$\frac{d^2u}{dx^2} = \frac{1}{x_0}\frac{d}{dx}\left(\frac{du}{d\xi}\right)$$

$$= \frac{1}{x_0^2}\frac{d}{d\xi}\left(\cancel{\frac{du}{dx}}\,\frac{du}{d\xi}\right)$$

$$= \frac{1}{x_0^2} \frac{d}{d\xi}\left(\frac{dy}{dx} x_0\right)$$

$$= \frac{1}{x_0^2} \frac{d}{d\xi}\left(\cancel{\frac{1}{x_0}} \frac{dy}{d\xi} \cancel{x_0}\right)$$

$$\boxed{\frac{d^2y}{dx^2} = \frac{1}{x_0^2} \frac{d^2y}{d\xi^2}}$$

Put in (1):

$$\frac{1}{x_0^2} \frac{d^2y}{d\xi^2} + \frac{2m}{\hbar^2}\left(\varepsilon_0 \epsilon - V_\xi\right) u = 0$$

$$V = \frac{1}{2} k x^2 + \frac{1}{3} b x^3$$

$$V = \frac{1}{2} k (x_0 \xi)^2 + \frac{1}{3} b (x_0 \xi)^3$$

$$V = \frac{1}{2} k x_0^2 \xi^2 + \frac{1}{3} b x_0^3 \xi^3$$

$$\frac{1}{x_0^2} \frac{d^2y}{d\xi^2} + \frac{2m}{\hbar^2}\left(\varepsilon_0 \epsilon - \frac{1}{2} k x_0^2 \xi^2 - \frac{1}{3} b x_0^3 \xi^3\right) u = 0$$

$$\frac{d^2y}{d\xi^2} + \frac{2m}{\hbar^2}\left(\varepsilon_0 \epsilon x_0^2 - \frac{1}{2} k \xi^2 x_0^4 - \frac{1}{3} b \xi^3 x_0^5\right) u = 0$$

Date :
Page No :

$$\frac{d^2 \psi}{d\xi^2} + \left[\frac{2m}{\hbar^2} x_0^2 \varepsilon_0 \epsilon - \frac{1}{2} k \times \frac{2m}{\hbar^2} \xi^2 x_0^4 - \frac{1}{3} b \xi^3 \times \frac{2m}{\hbar^2} x_0^5\right] \psi = 0$$

So, $\frac{2m x_0^2 \varepsilon_0}{\hbar^2} = 1$

& $\frac{mk x_0^4}{\hbar^2} = 1$

$$\boxed{\begin{aligned} x_0 &= \left(\frac{\hbar^2}{mk}\right)^{1/4} \\ x_0^2 &= \left(\frac{\hbar^2}{mk}\right)^{1/2} \end{aligned}}$$

& $\varepsilon_0 = \frac{\hbar^2}{2m x_0^2}$

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

$\varepsilon_0 = \frac{\hbar \sqrt{k}}{2\sqrt{m}}$

$$\boxed{\varepsilon_0 = \frac{\omega \hbar}{2}}$$

Date :
Page No. :

Also, $\dfrac{2mb}{3\hbar^2} x_0^5 \ll 1$

$$b = \frac{\hbar^2}{2m x_0^5}$$

$$= \frac{\hbar^2}{2m}\left(\frac{mk}{\hbar^2}\right)^{5/4}$$

$$= \frac{\hbar^{2-\frac{5}{2}}}{2m}(mk)^{5/4}$$

$$= \frac{\hbar^{-\frac{1}{2}}}{2} m^{1/4} k^{5/4}$$

$$= \frac{2}{\sqrt{\hbar}}\left(mk^5\right)^{1/4}$$

$$\frac{2mb}{3\hbar^2} x_0^4 x_0 \ll 1$$

$$\frac{2mb}{3\hbar^2} \times \frac{\hbar^2}{mk} x_0 \ll 1$$

$$= \frac{2}{3}\frac{b x_0}{k} \ll 1$$

$$\frac{d^2u}{d\xi^2} + \left[\varepsilon - \xi^2 - \frac{2}{3}\frac{b x_0}{k}\xi^3\right]u = 0$$

$$\cancel{k = \mu\omega^2}$$

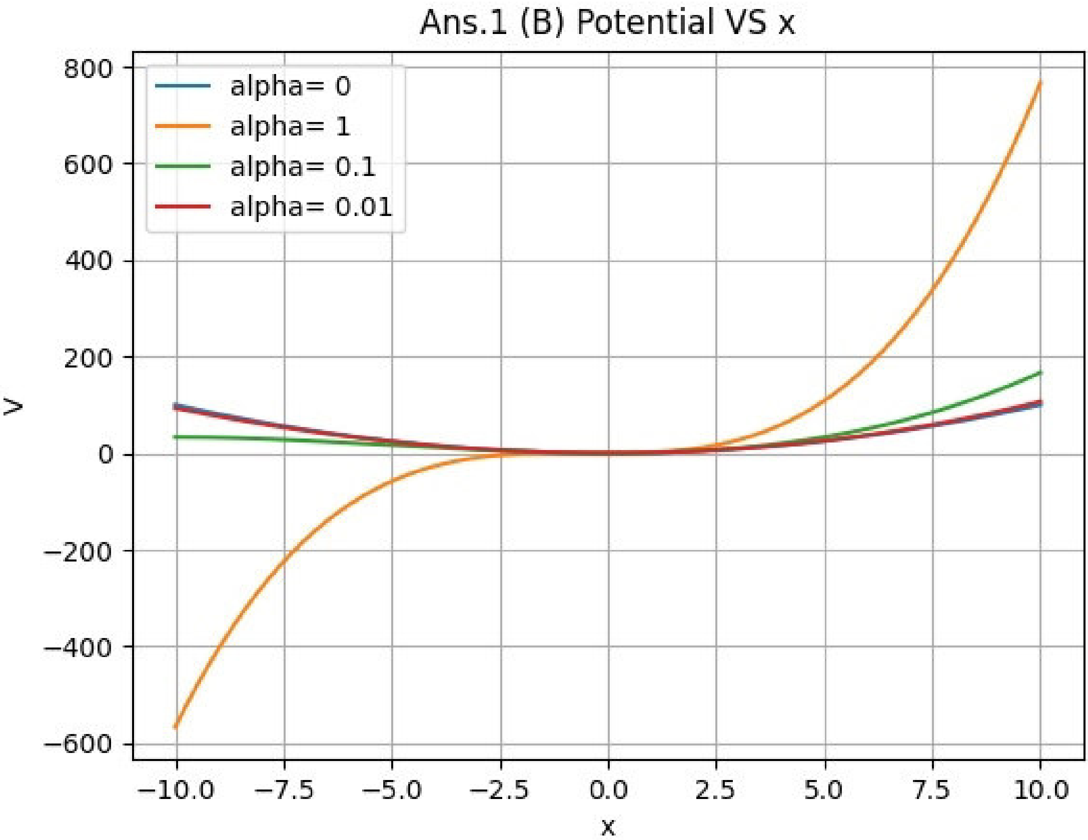
$$\frac{d^2u}{d\xi^2} + \left[\varepsilon - \xi^2 - \frac{2}{3}\alpha\xi^3\right]u = 0$$

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

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

$$-\left(\frac{u_{i+1} - 2u_i + u_{i-1}}{(\Delta\xi)^2}\right) + (V_i)\,u_i = \varepsilon u_i$$

$$\frac{-1}{(\Delta\xi)^2}\begin{bmatrix} 1 & -2 & 1 & \cdots & \\ 0 & 1 & -2 & 1 & \\ 0 & & & & \\ 1 & & & & \\ 0 & 0 & \cdots & 1 & -2 \end{bmatrix}$$


Ans.1 (B) Potential VS x
alpha= 0
alpha= 1
alpha= 0.1
alpha= 0.01
800
600
400
200
0
−200
−400
−600
V
−10.0
−7.5
−5.0
−2.5
0.0
2.5
5.0
7.5
10.0
x

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

def matrix(a, b, n, l,alpha):
    x = np.arange(a, b, n)
    # print(x)
    h = x[1] - x[0]
    u = np.zeros(shape=(len(x), len(x)))
    V = np.zeros(shape=(len(x), len(x)))
    for i in range(1, len(x) - 1):
        for j in range(1, len(x)):
            if i == j:
                u[i][j] = (2 / h ** 2)
                V[i][j] = x[i]**2 + (2/3)*(alpha*(x[i])**
3)
            elif i == j + 1:
                u[i][j] = -1 / h ** 2
            elif i == j - 1:
                u[i][j] = -1 / h ** 2
    return u + V, x

def plot(i, l, power,ratio):
    H, x = matrix(-5, 5, 0.01, l,ratio)
    u = eigh(H)[1][:, i+2]
    # print(u)
    # NORMALIZATION
    c = integrate.simps(u ** 2, x)
    N = u / np.sqrt(c)
    if power==2:
        plt.ylabel("Ψ square")
    else:
        plt.ylabel("Ψ")
    plt.xlabel('x')
```

```
    plt.plot(x, N ** power, label='for alpha='+str(
ratio))
    plt.legend()

def eigen(a, b, h, l,ratio, i):
    H, x = matrix(a, b, h, l,ratio)
    u = eigh(H)[0][i+2]
    v = eigh(H)[1][:, i]
    return u

x=np.linspace(-10,10,200)
alpha=[0,1,10**(-1),10**(-2)]
for i in alpha:
    V=x**2 + (2/3)*(i*(x)**3)
    plt.plot(x,V,label='alpha= '+str(i))
plt.grid()
plt.legend()
plt.xlabel('x')
plt.ylabel('V')
plt.title('Ans.1 (B) Potential VS x')
plt.savefig('Potential.jpg')
plt.show()
# A,B

for j in range(0,11):
    En_calc=[]
    En_analy=[]
    alpha=[]
    for i in [0,1,10**(-1),10**(-2),10**(-3),10**(-
4)]:
        alpha.append(i)
        energy=eigen(-20, 20, 0.1, 0, i, j)
        analytic= (2*j + 1) - (1/8)*(i**2)*(15*(2*j
 + 1)**2 + 7)
        En_calc.append(energy)
        En_analy.append(analytic)
```

```
    print('Energy eigen values For n=',j)
    print(pd.DataFrame({'alpha':alpha,'Calculated'
:En_calc,'Analytic': En_analy}))
    print(
"==============================
==============================")

#C,D

En=[]
ratio=[0,1,10**(-1),10**(-2),10**(-3),10**(-4)]
n=[0,1,2,3,4,5,6,7,8,9,10]
for j in ratio:
    E=[]
    for i in n:
        energy = eigen(-20, 20, 0.1, 0, j, i)
        E.append(energy)
    En.append(E)
p=0
for i in En:
    plt.scatter(n,i)
    plt.grid()
    plt.xlabel('n (states)')
    plt.ylabel('Energy eigen value')
    plt.title('For alpha= '+str(alpha[p]))
    plt.savefig('alpha=' + str(alpha[p])+'.jpg')
    plt.show()
    p+=1
n=[0,1,2,3,4,5]
ratio=[0,1,10**(-1),10**(-2)]
for j in n:
    E=[]
    for i in ratio:
        plot(j,0,1,i)
    plt.title('For n='+str(j)+' Ψ VS x')
    plt.grid()
```

```
    plt.savefig('n='+str(j)+'_power1')
    plt.show()
    for i in ratio:
        plot(j,0,2,i)
    plt.title('For n='+str(j)+' Ψ square VS x')
    plt.grid()
    plt.savefig('n=' + str(j) + '_power2')
    plt.show()
```

```
C:\Users\anura\AppData\Local\Programs\Python\
Python38\python.exe E:/SEM-5/A13/A13.1.py
Energy eigen values For n= 0
   alpha   Calculated  Analytic
0  0.0000     0.999375  1.000000
1  1.0000 -4520.279499 -1.750000
2  0.1000   -73.638172  0.972500
3  0.0100     0.999344  0.999725
4  0.0010     0.999374  0.999997
5  0.0001     0.999375  1.000000
==================================
=========================
Energy eigen values For n= 1
   alpha   Calculated   Analytic
0  0.0000     2.996871   3.000000
1  1.0000 -4438.994397 -14.750000
2  0.1000   -61.332771   2.822500
3  0.0100     2.996675   2.998225
4  0.0010     2.996870   2.999982
5  0.0001     2.996871   3.000000
==================================
=========================
Energy eigen values For n= 2
   alpha   Calculated   Analytic
0  0.0000     4.991861   5.000000
1  1.0000 -4364.710601 -42.750000
2  0.1000   -50.544683   4.522500
3  0.0100     4.991333   4.995225
4  0.0010     4.991856   4.999952
5  0.0001     4.991861   5.000000
==================================
=========================
Energy eigen values For n= 3
   alpha   Calculated   Analytic
0  0.0000     6.984339   7.000000
1  1.0000 -4292.732574 -85.750000
```

```
2  0.1000   -40.893712   6.072500
3  0.0100     6.983316   6.990725
4  0.0010     6.984329   6.999907
5  0.0001     6.984339   6.999999
===================================
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Energy eigen values For n= 4
   alpha   Calculated    Analytic
0  0.0000     8.974301    9.000000
1  1.0000 -4221.723043 -143.750000
2  0.1000   -32.149789    7.472500
3  0.0100     8.972619    8.984725
4  0.0010     8.974284    8.999847
5  0.0001     8.974300    8.999998
===================================
======================
Energy eigen values For n= 5
   alpha   Calculated    Analytic
0  0.0000    10.961741   11.000000
1  1.0000 -4151.483667 -216.750000
2  0.1000   -24.160727    8.722500
3  0.0100    10.959238   10.977225
4  0.0010    10.961716   10.999772
5  0.0001    10.961740   10.999998
===================================
======================
Energy eigen values For n= 6
   alpha   Calculated    Analytic
0  0.0000    12.946654   13.000000
1  1.0000 -4081.993823 -304.750000
2  0.1000   -16.819822    9.822500
3  0.0100    12.943169   12.968225
4  0.0010    12.946620   12.999682
5  0.0001    12.946654   12.999997
===================================
======================
```

Energy eigen values For n= 7

	alpha	Calculated	Analytic
0	0.0000	14.929037	15.000000
1	1.0000	-4013.248564	-407.750000
2	0.1000	-10.049296	10.772500
3	0.0100	14.924409	14.957725
4	0.0010	14.928991	14.999577
5	0.0001	14.929037	14.999996

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Energy eigen values For n= 8

	alpha	Calculated	Analytic
0	0.0000	16.908884	17.000000
1	1.0000	-3945.243862	-525.750000
2	0.1000	-3.791071	11.572500
3	0.0100	16.902954	16.945725
4	0.0010	16.908824	16.999457
5	0.0001	16.908883	16.999995

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Energy eigen values For n= 9

	alpha	Calculated	Analytic
0	0.0000	18.886189	19.000000
1	1.0000	-3877.975731	-658.750000
2	0.1000	0.000000	12.222500
3	0.0100	18.878800	18.932225
4	0.0010	18.886115	18.999322
5	0.0001	18.886189	18.999993

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Energy eigen values For n= 10

	alpha	Calculated	Analytic
0	0.0000	20.860949	21.000000
1	1.0000	-3811.440188	-806.750000
2	0.1000	0.000000	12.722500
3	0.0100	20.851942	20.917225

```
4  0.0010    20.860859   20.999172
5  0.0001    20.860948   20.999992
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Process finished with exit code 0
```
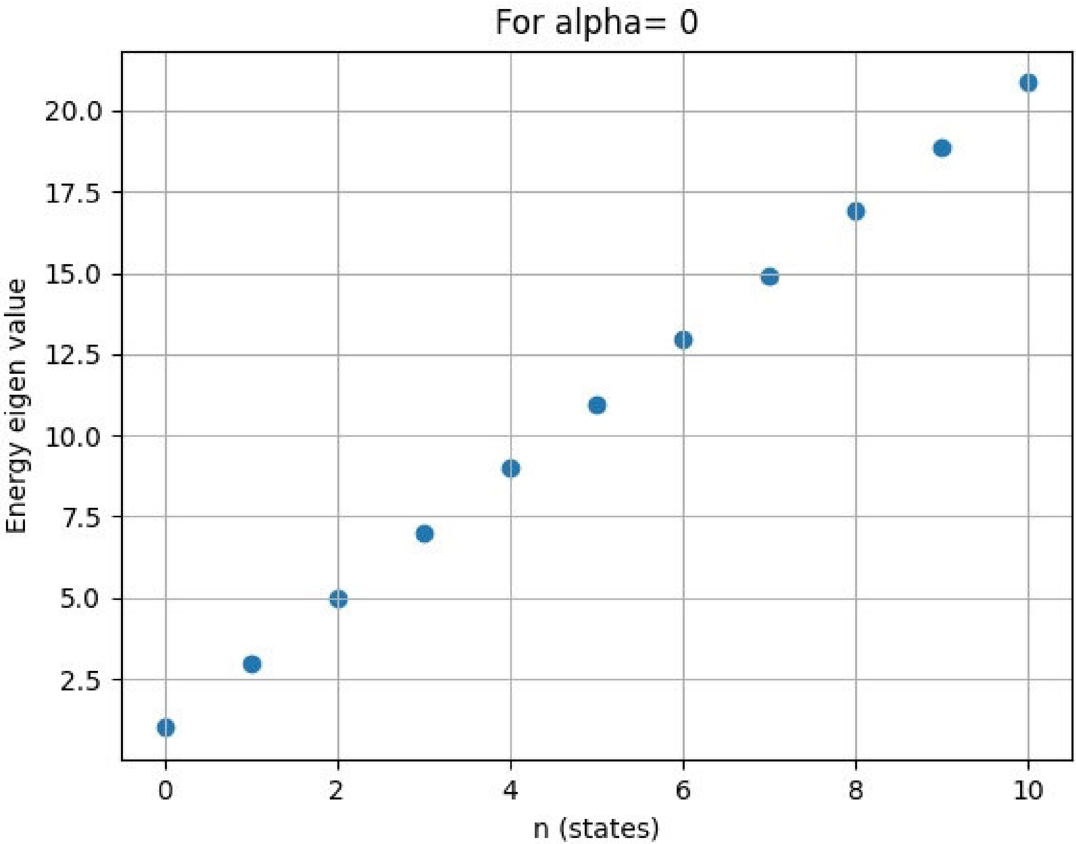
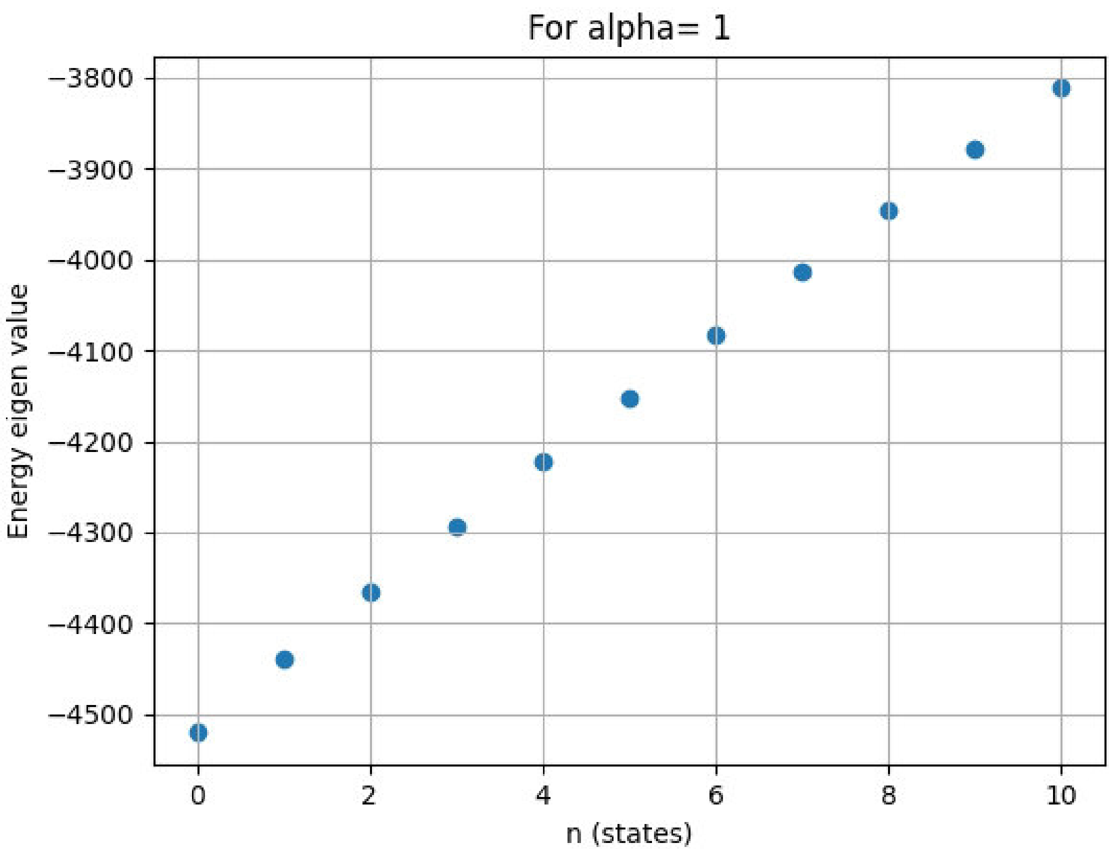
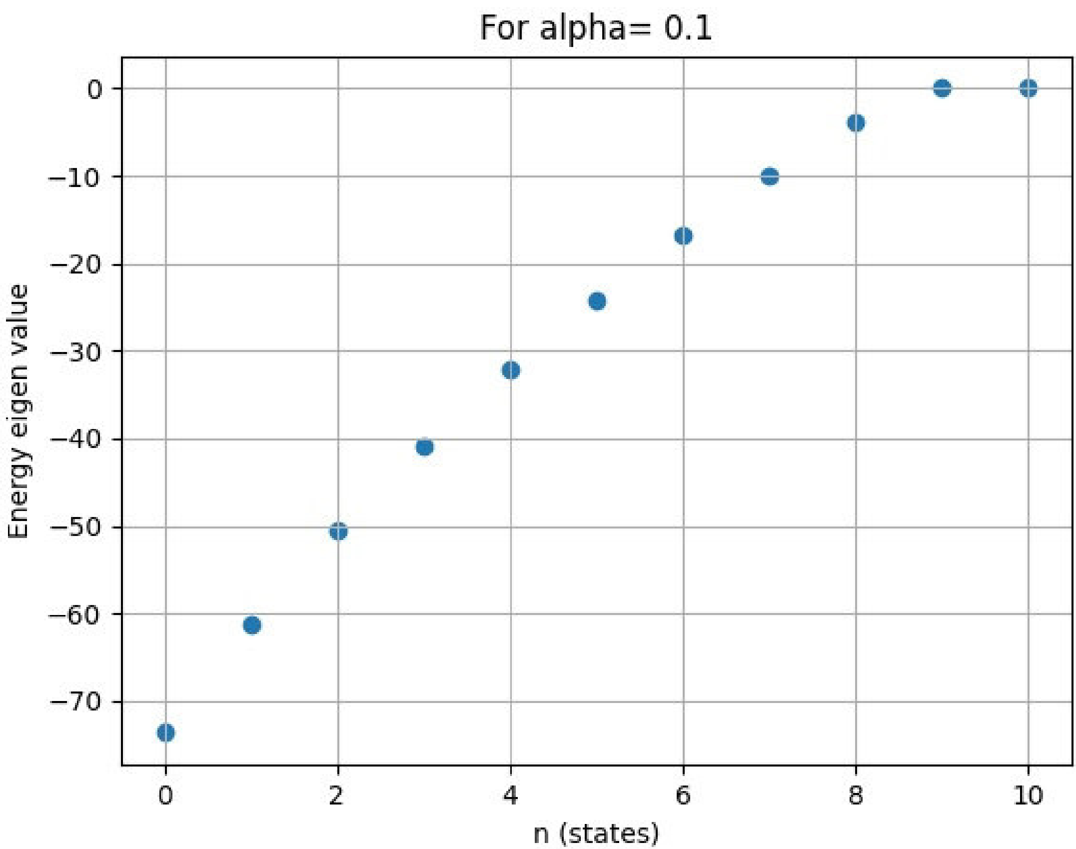
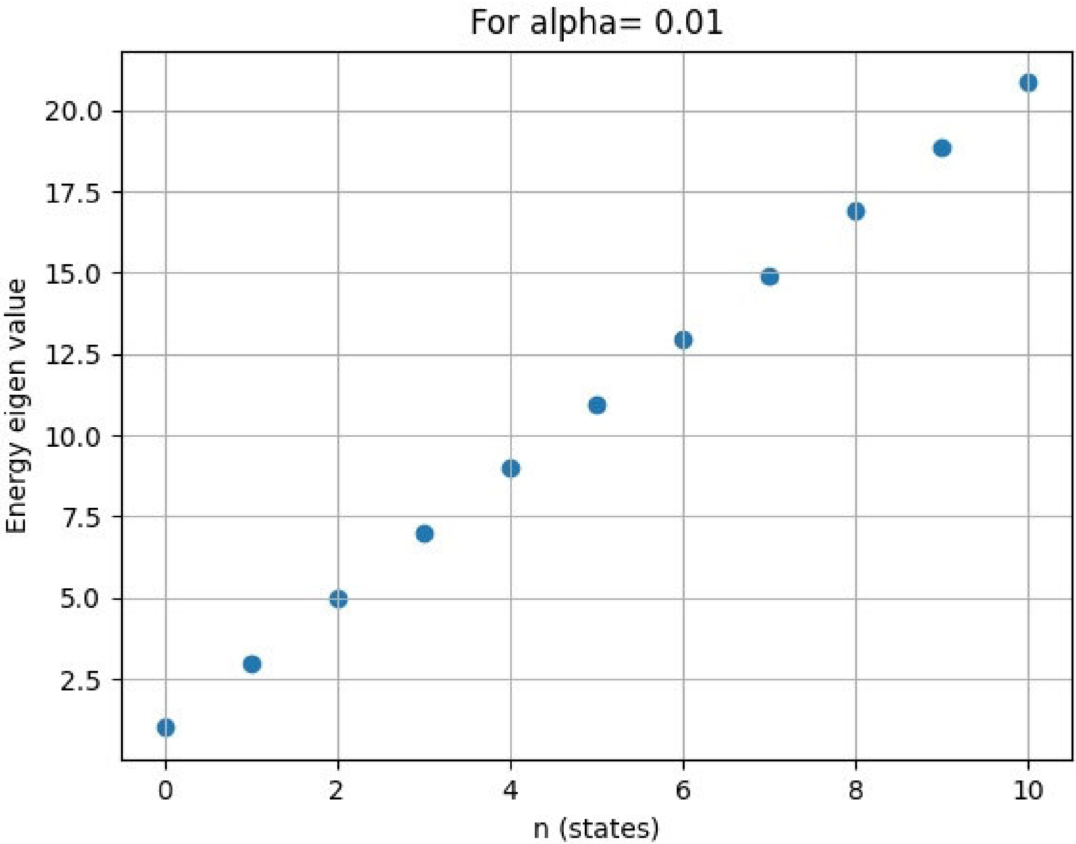
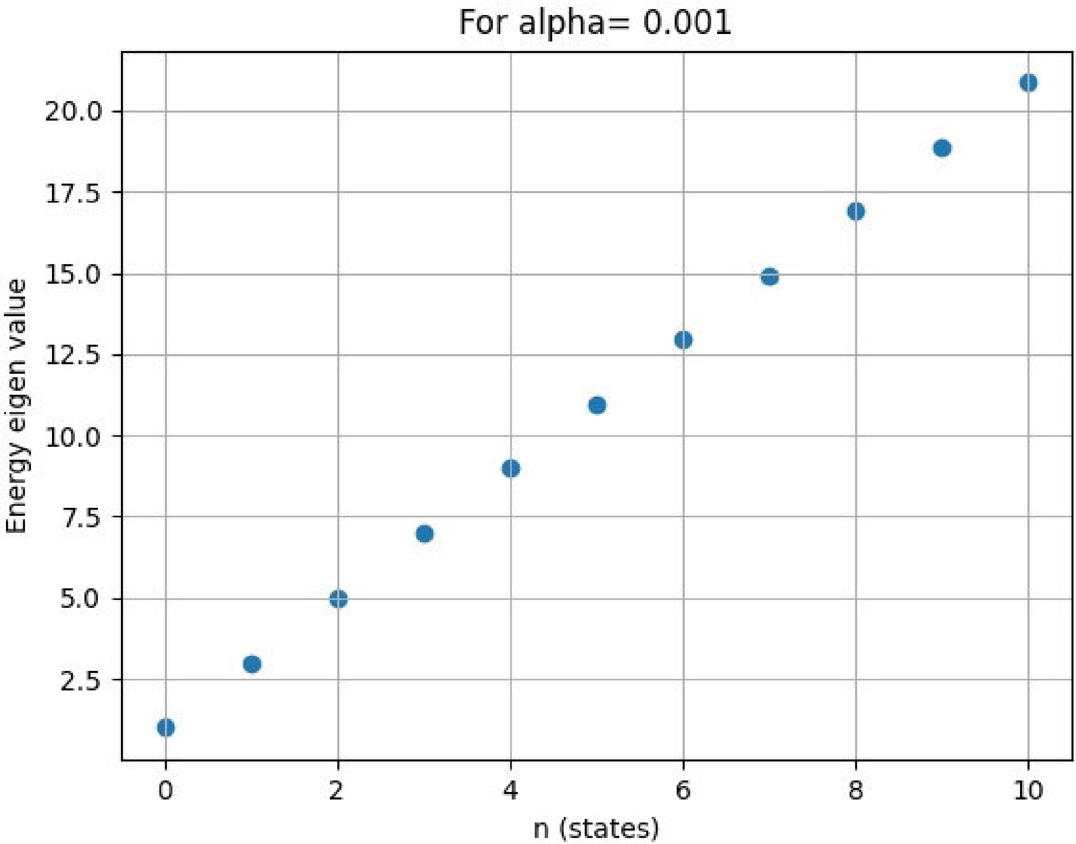
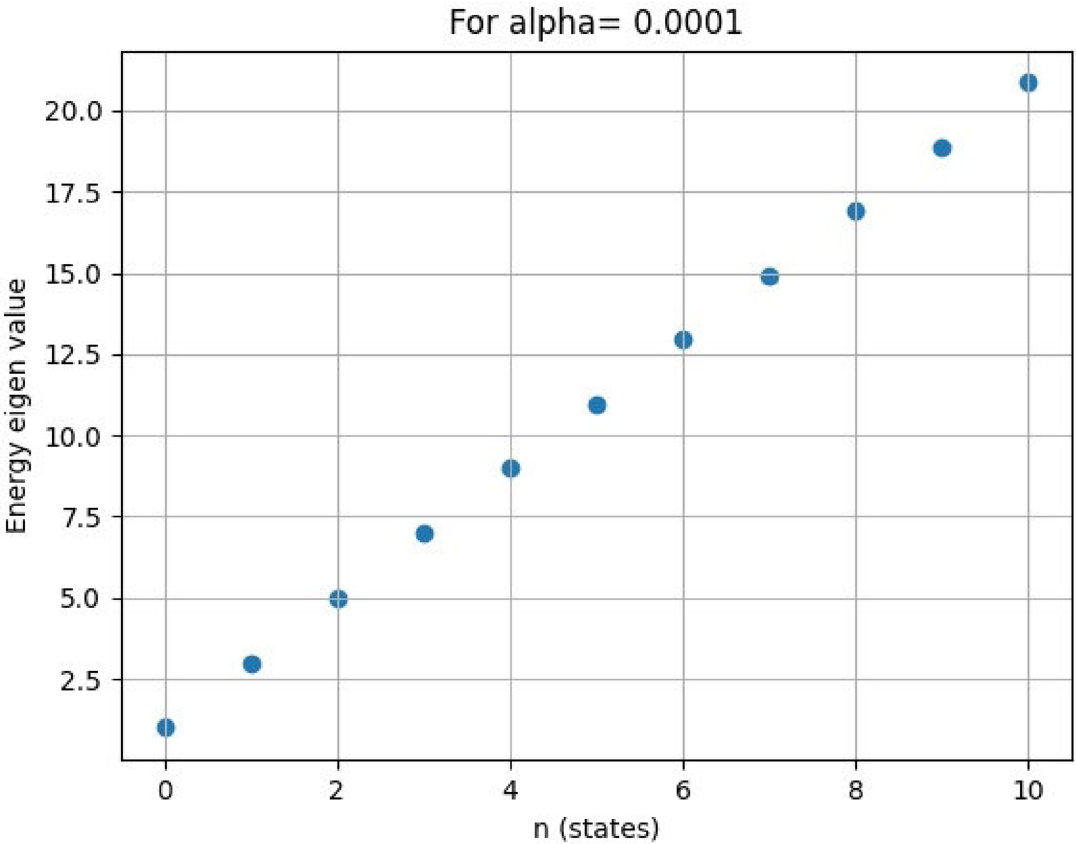


For alpha= 0
Energy eigen value
n (states)
20.0
17.5
15.0
12.5
10.0
7.5
5.0
2.5
0
2
4
6
8
10

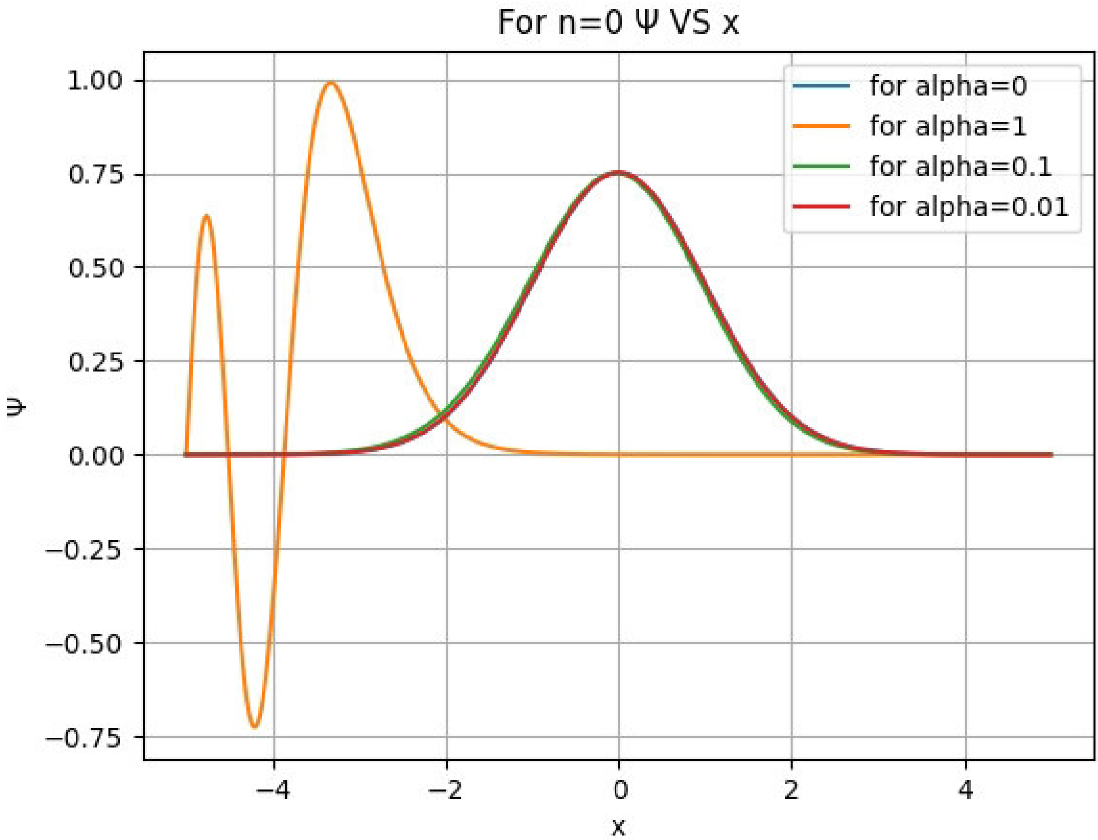

For alpha= 1
Energy eigen value
−3800
−3900
−4000
−4100
−4200
−4300
−4400
−4500
0
2
4
6
8
10
n (states)


For alpha= 0.1
Energy eigen value
n (states)
0
−10
−20
−30
−40
−50
−60
−70
0
2
4
6
8
10

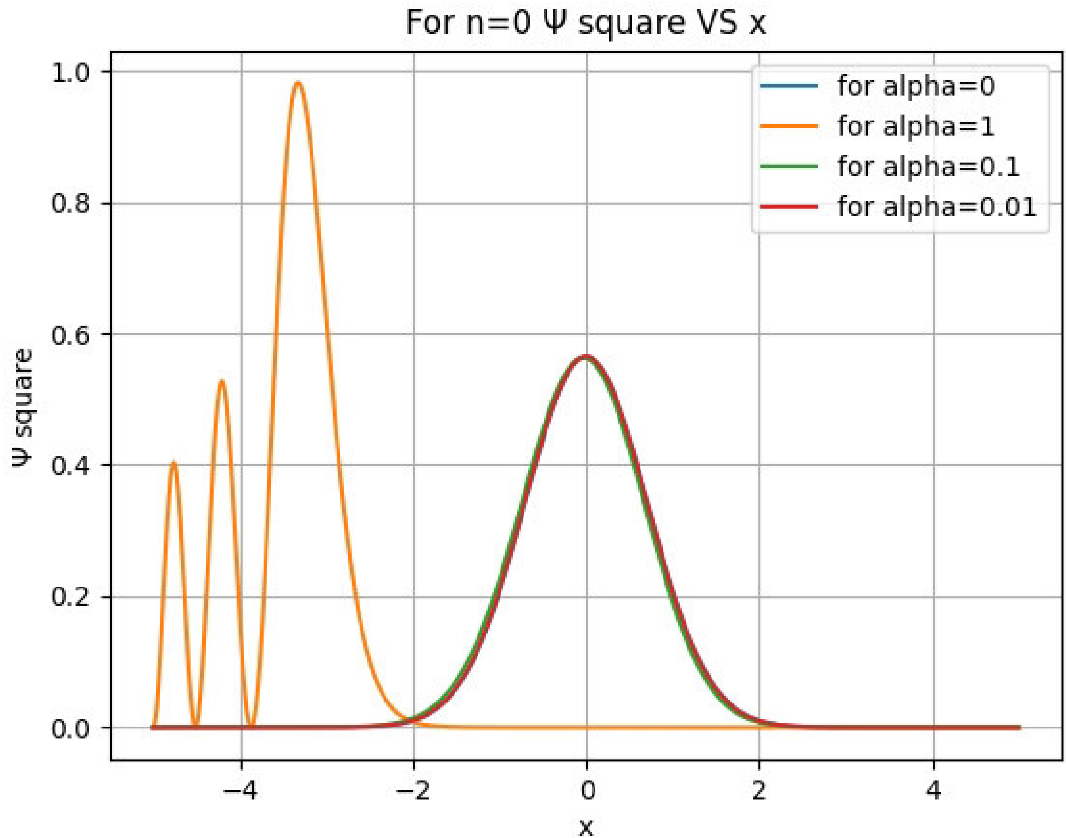

For alpha= 0.01
Energy eigen value
n (states)
0
2
4
6
8
10
2.5
5.0
7.5
10.0
12.5
15.0
17.5
20.0

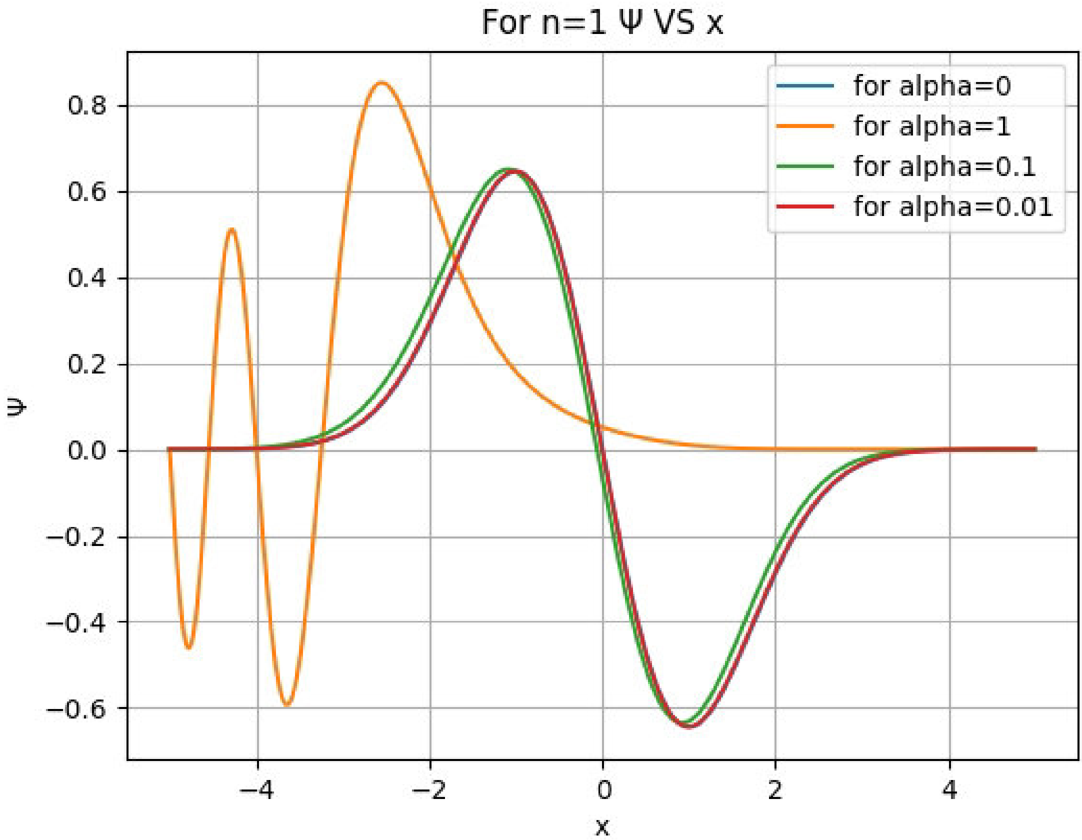

For alpha= 0.001
Energy eigen value
n (states)
0
2
4
6
8
10
2.5
5.0
7.5
10.0
12.5
15.0
17.5
20.0


For alpha= 0.0001
Energy eigen value
n (states)
20.0
17.5
15.0
12.5
10.0
7.5
5.0
2.5
0
2
4
6
8
10

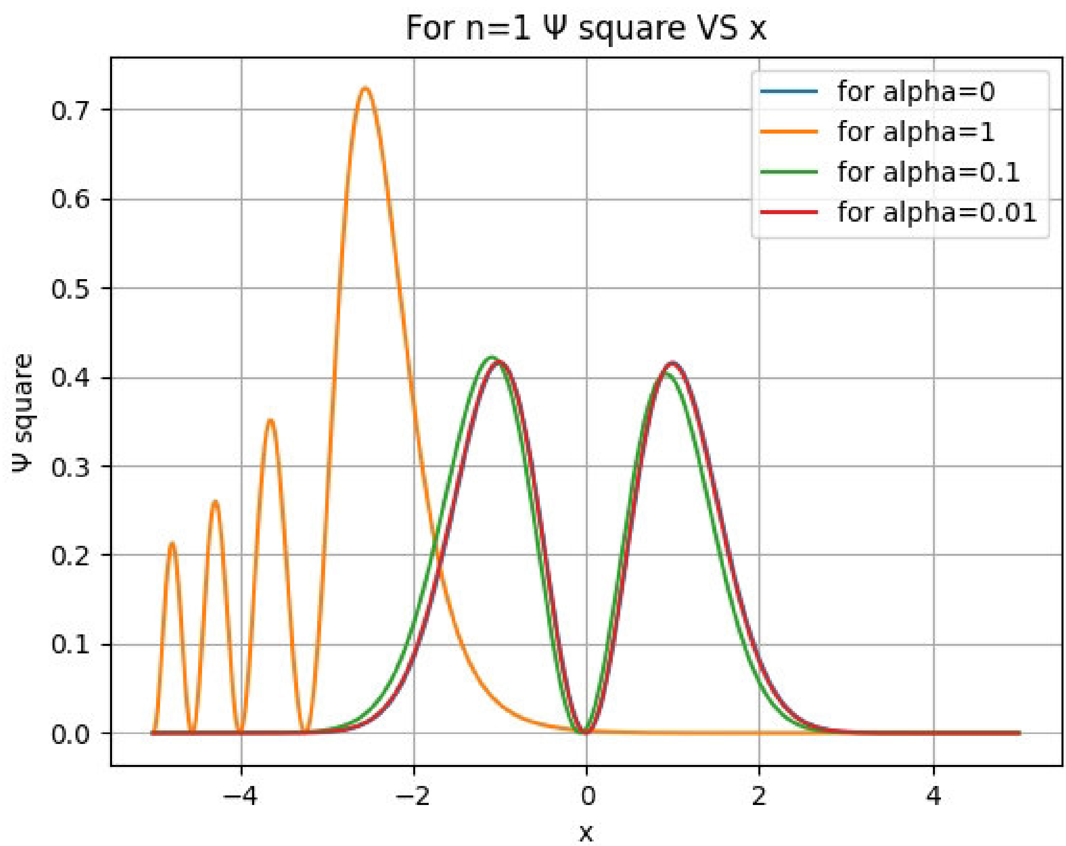


For n=0 Ψ VS x
for alpha=0
for alpha=1
for alpha=0.1
for alpha=0.01
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
Ψ
−4
−2
0
2
4
x

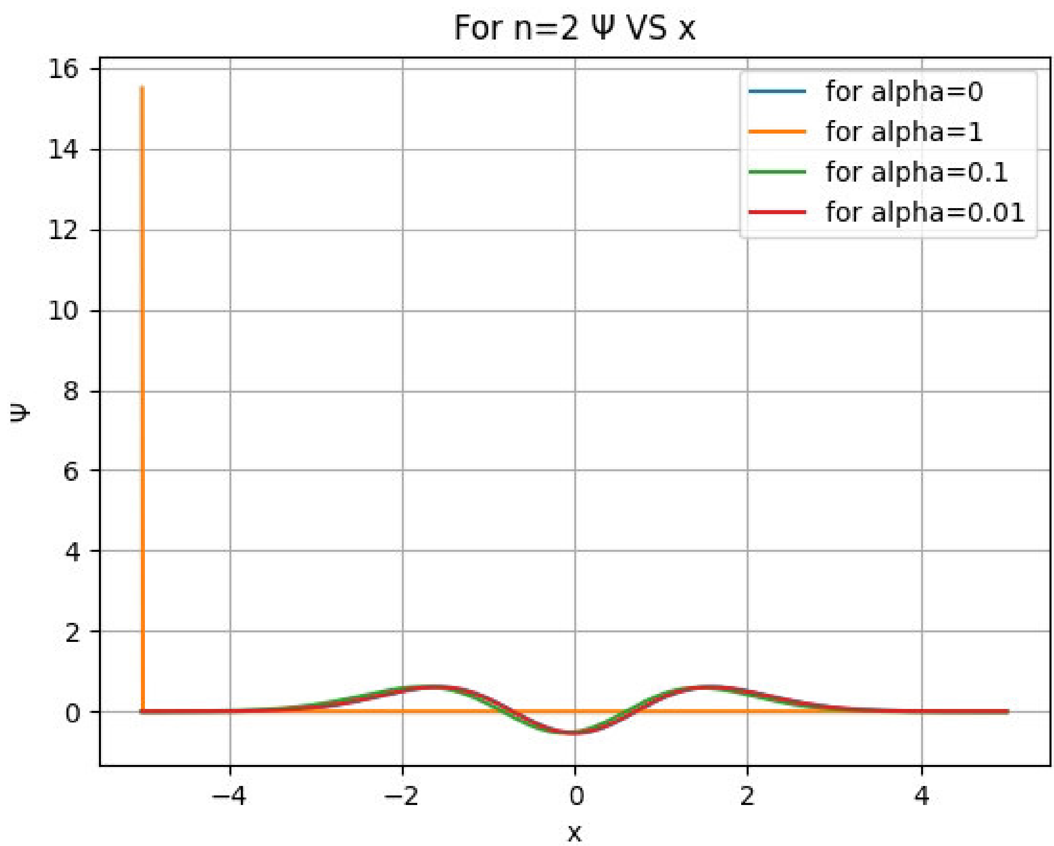

For n=0 Ψ square VS x
for alpha=0
for alpha=1
for alpha=0.1
for alpha=0.01
1.0
0.8
0.6
0.4
0.2
0.0
Ψ square
−4
−2
0
2
4
x

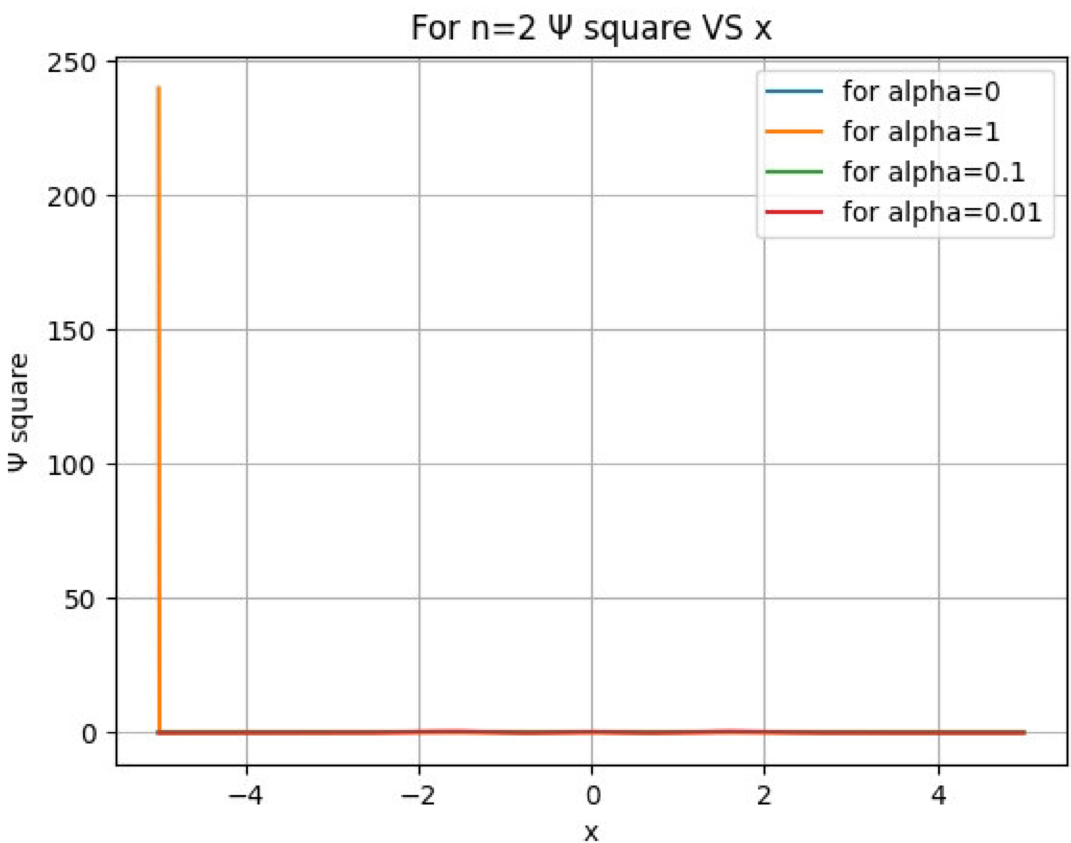


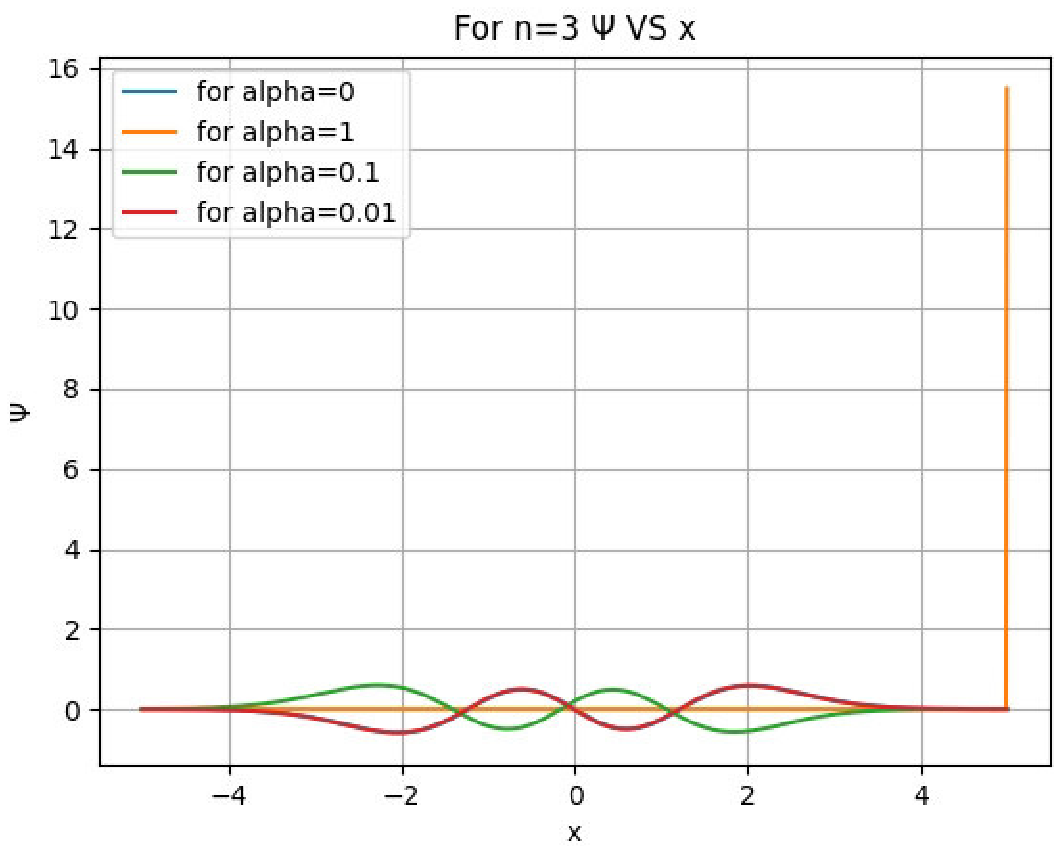
For n=1 Ψ VS x
for alpha=0
for alpha=1
for alpha=0.1
for alpha=0.01
Ψ
x
0.8
0.6
0.4
0.2
0.0
−0.2
−0.4
−0.6
−4
−2
0
2
4



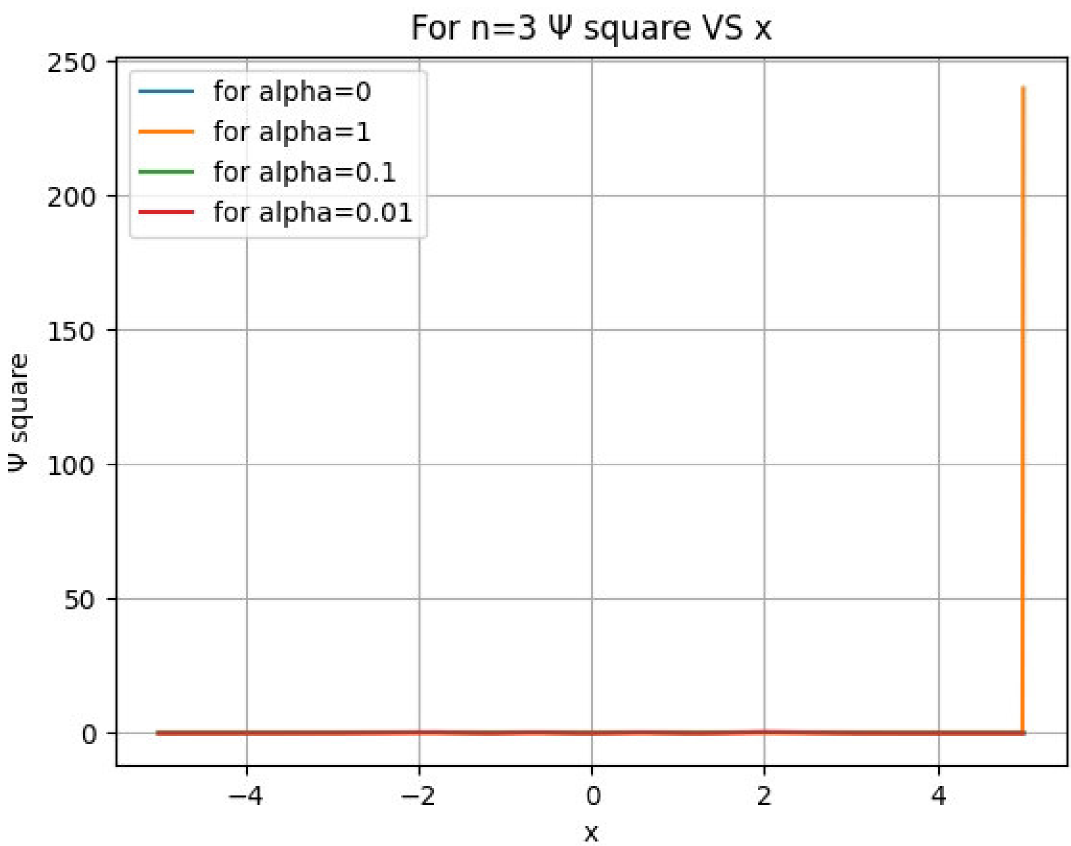
For n=1 Ψ square VS x
for alpha=0
for alpha=1
for alpha=0.1
for alpha=0.01
Ψ square
x
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
−4
−2
0
2
4

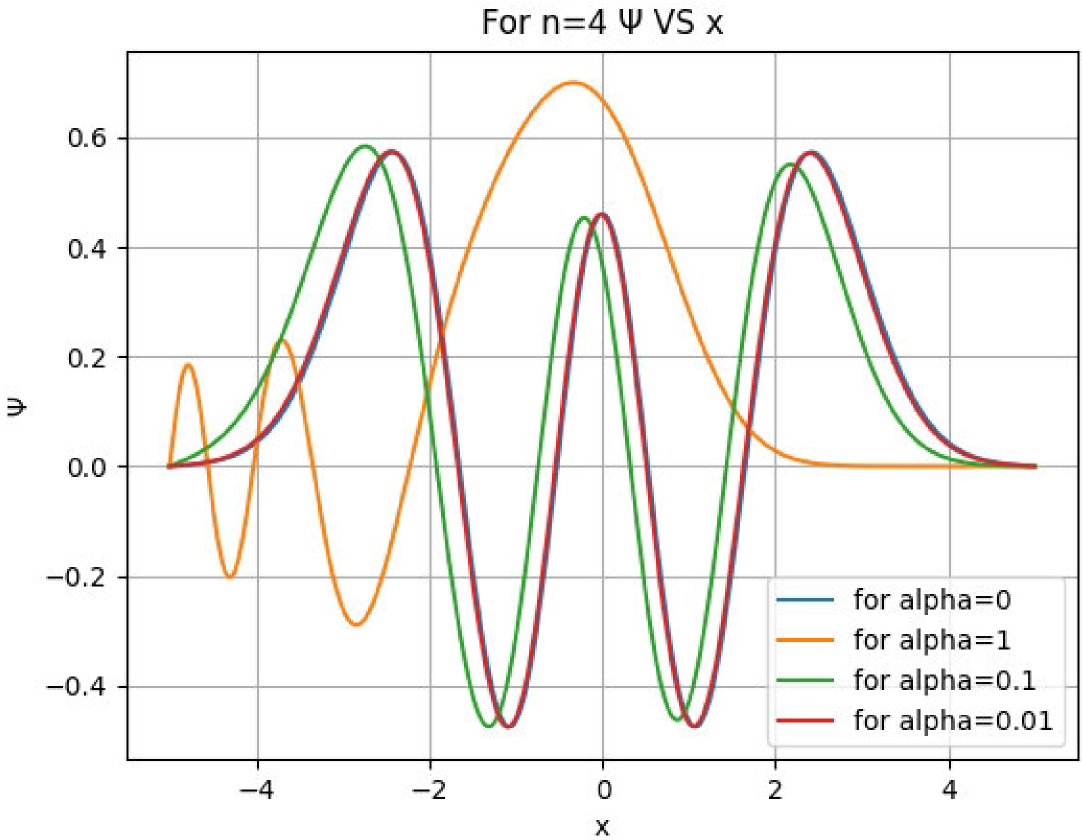

For n=2 Ψ VS x
for alpha=0
for alpha=1
for alpha=0.1
for alpha=0.01
Ψ
x
16
14
12
10
8
6
4
2
0
−4
−2
0
2
4


For n=2 Ψ square VS x
Ψ square
x
250
200
150
100
50
0
−4
−2
0
2
4
for alpha=0
for alpha=1
for alpha=0.1
for alpha=0.01

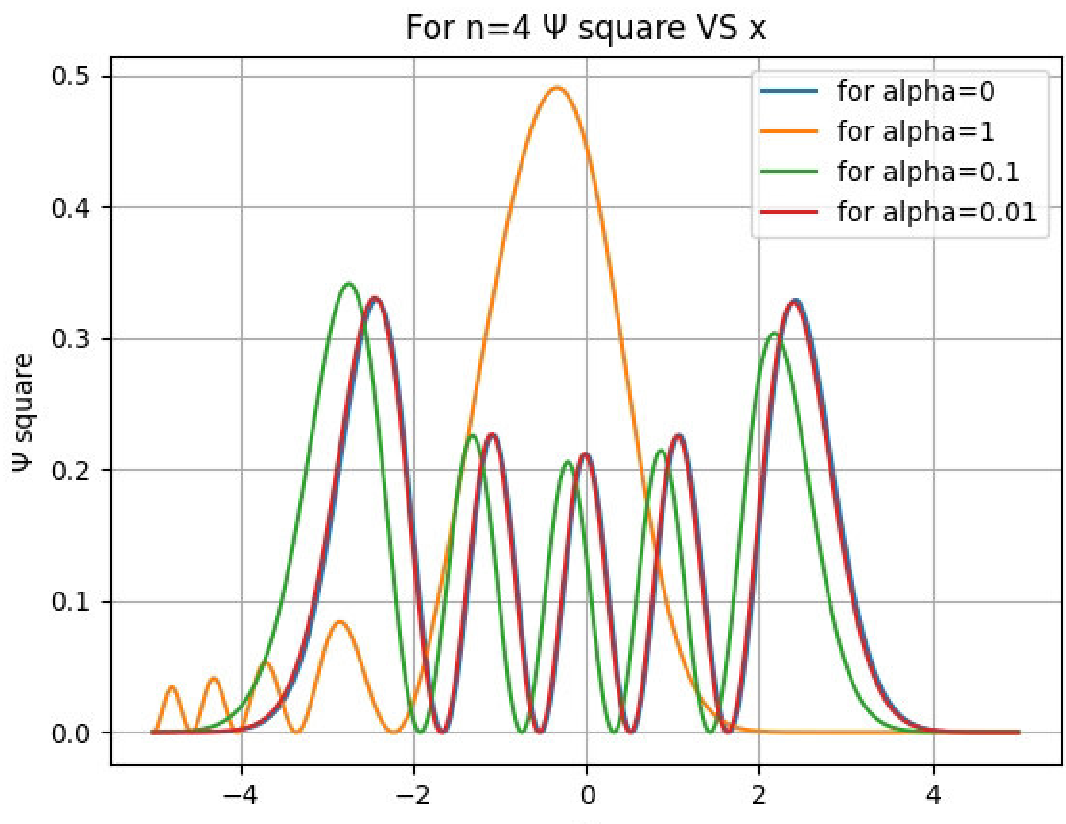


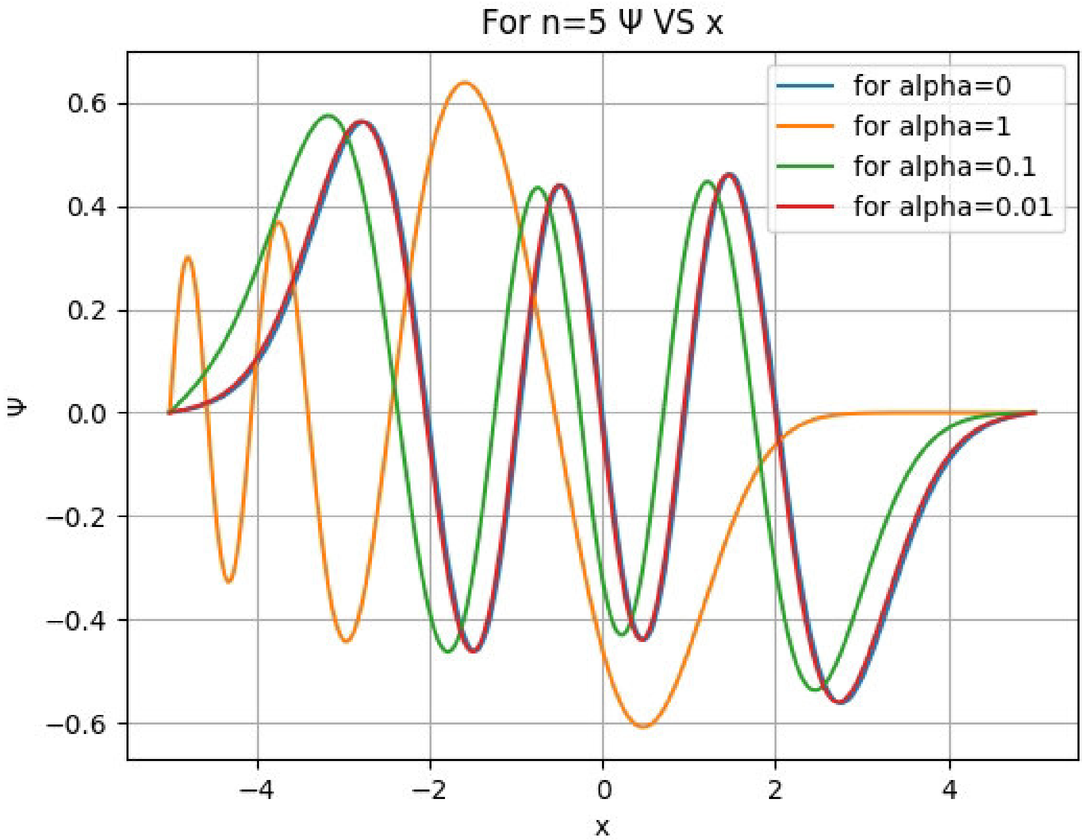
For n=3 Ψ VS x
for alpha=0
for alpha=1
for alpha=0.1
for alpha=0.01
Ψ
x
16
14
12
10
8
6
4
2
0
−4
−2
0
2
4


For n=3 Ψ square VS x
for alpha=0
for alpha=1
for alpha=0.1
for alpha=0.01
Ψ square
x
250
200
150
100
50
0
−4
−2
0
2
4

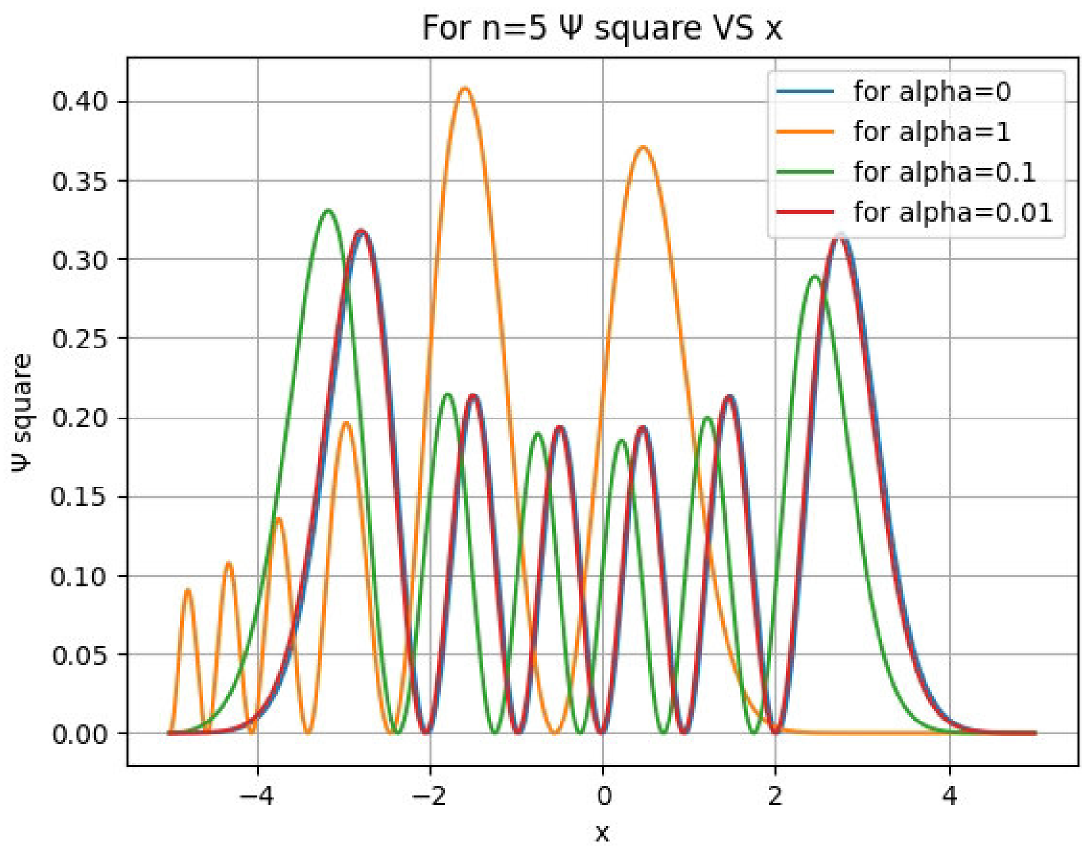


For n=4 Ψ VS x
Ψ
x
0.6
0.4
0.2
0.0
−0.2
−0.4
−4
−2
0
2
4
for alpha=0
for alpha=1
for alpha=0.1
for alpha=0.01


For n=4 Ψ square VS x
for alpha=0
for alpha=1
for alpha=0.1
for alpha=0.01
Ψ square
x
0.5
0.4
0.3
0.2
0.1
0.0
−4
−2
0
2
4



For n=5 Ψ VS x
for alpha=0
for alpha=1
for alpha=0.1
for alpha=0.01
Ψ
x
0.6
0.4
0.2
0.0
−0.2
−0.4
−0.6
−4
−2
0
2
4


For n=5 Ψ square VS x
for alpha=0
for alpha=1
for alpha=0.1
for alpha=0.01
Ψ square
x
0.00
0.05
0.10
0.15
0.20
0.25
0.30
0.35
0.40
−4
−2
0
2
4