```python
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#rollno : 2020PHY1122

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

def fin_diff(a,b,n):
    h = (b-a)/(n-1)  #n is number of grid points

    K,V = np.zeros((n,n)),np.zeros((n,n))

    X = np.linspace(a,b,n)

    K[0,0] = -2;K[0,1] = 1
    K[n-1,n-1] = -2;K[n-1,n-2] = 1

    for i in range(1,n-1):
        K[i,i]=-2
        K[i,i-1]=1
        K[i,i+1]=1

    H = (-1*K)/(h**2) + V

    U = eigh(H)[1]
    e = eigh(H)[0]

    return [e,U,X]
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def MySimp(x,y):  #x here is the array of independent variable  and y for dependent variable
    # calculating step size
    h = abs((x[-1] - x[0]) / len(x))

    simpint = y[0] + y[-1]

    for i in range(1,len(x)):

        if i%2 == 0:
            simpint = simpint + 2 * y[i]
        else:
            simpint = simpint + 4 * y[i]

    # multiply h/2 with the obtained integration to get Simpson integration
    simpint =simpint * h/3

    return simpint

def normalize(wavefx,wavefy,int_method = MySimp):  #this function returns list including normalisation constant and
                                                 #normalised eigen function
    I = int_method(wavefx,wavefy**2)
    A = (I)**(-1/2)

    return [A,A*wavefy]
```

```
def plots(x,y1,y2,ylabel,title,num,color = None): #num defines if there would be only one plot or more

    if num == 1:
        plt.plot(x, y2,linewidth = 2.5, label='analytical',c = 'b',ls = 'dashed')
        plt.scatter(x, y1,s = 20 ,label='computed',c = 'r')
    else :
        for i in range(len(y1)):
            plt.plot(x, y2[i], label='analytical n = '+ str(i),c = color[i][0],ls = 'dashed')
            plt.scatter(x, y1[i],s=5, label='computed n = '+ str(i),c=color[i][1])
    plt.grid()
    plt.xlabel('x')
    plt.ylabel(ylabel)
    plt.title(title)
    plt.legend()
    plt.show()

#PROGRAMMING

sol = fin_diff(-0.5, 0.5, 1000)

print("THE FIRST 10 EIGEN VALUES COMPUTED USING FINITE DIFFERENCE METHOD ARE : ")

anal_e = []

for i in range(1,11):
    anal_e.append((i*np.pi)**2)

print(pd.DataFrame({'COMPUTED e':sol[0][:10],'ANALYTICAL e':anal_e}))

U_sq_list , Anal_U_sq_list = [],[]   #these lists will carry the square of values for density plot

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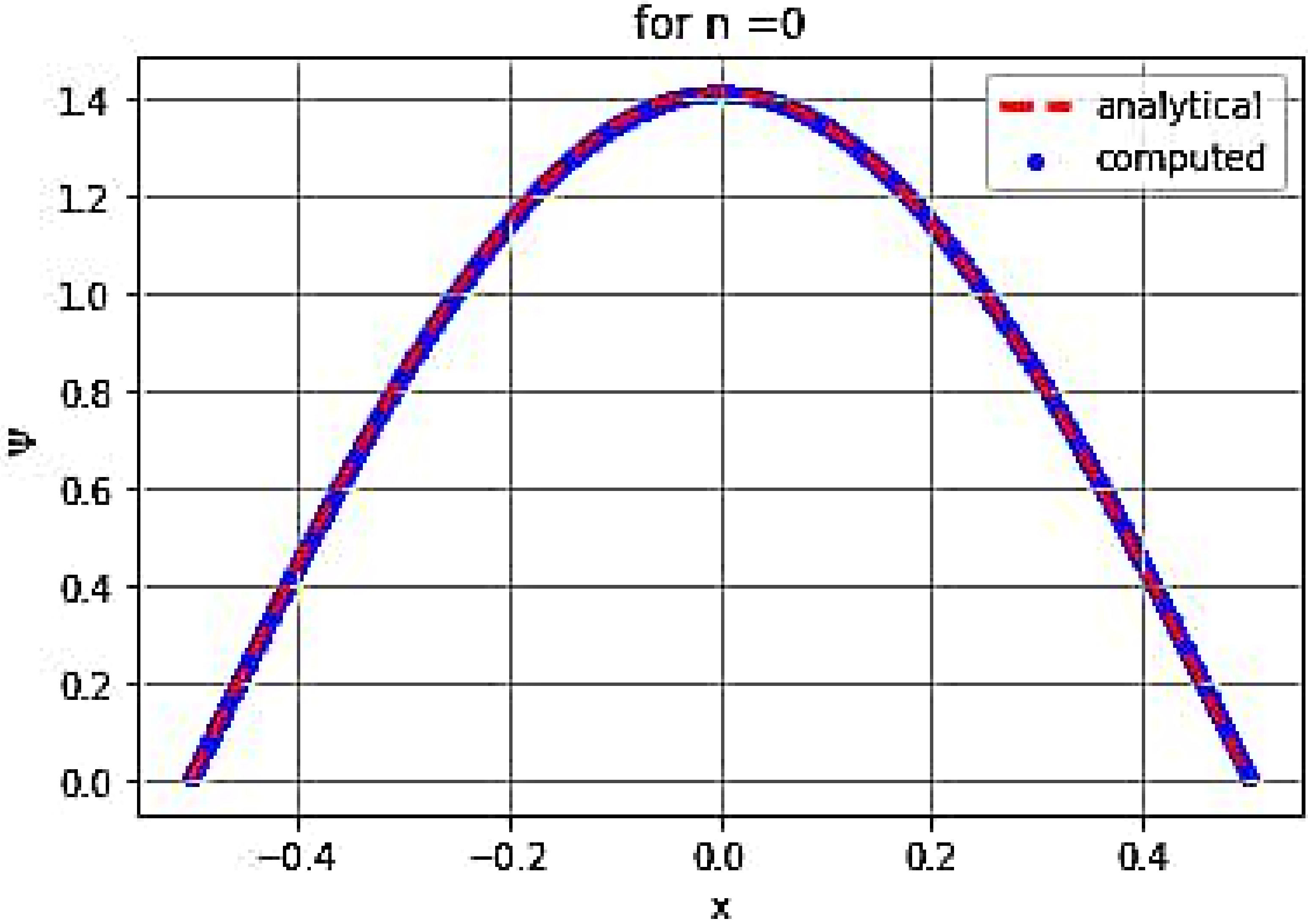
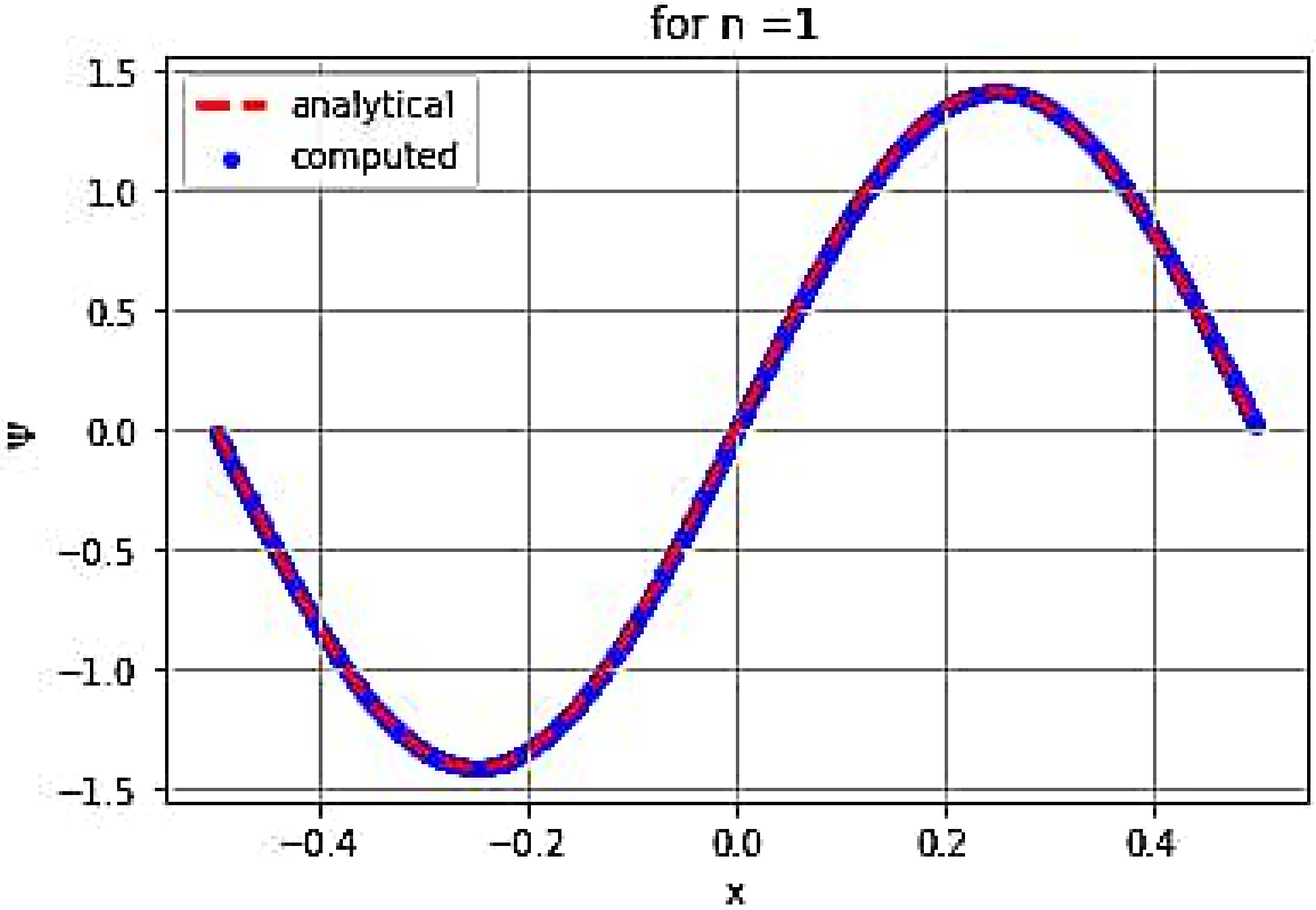
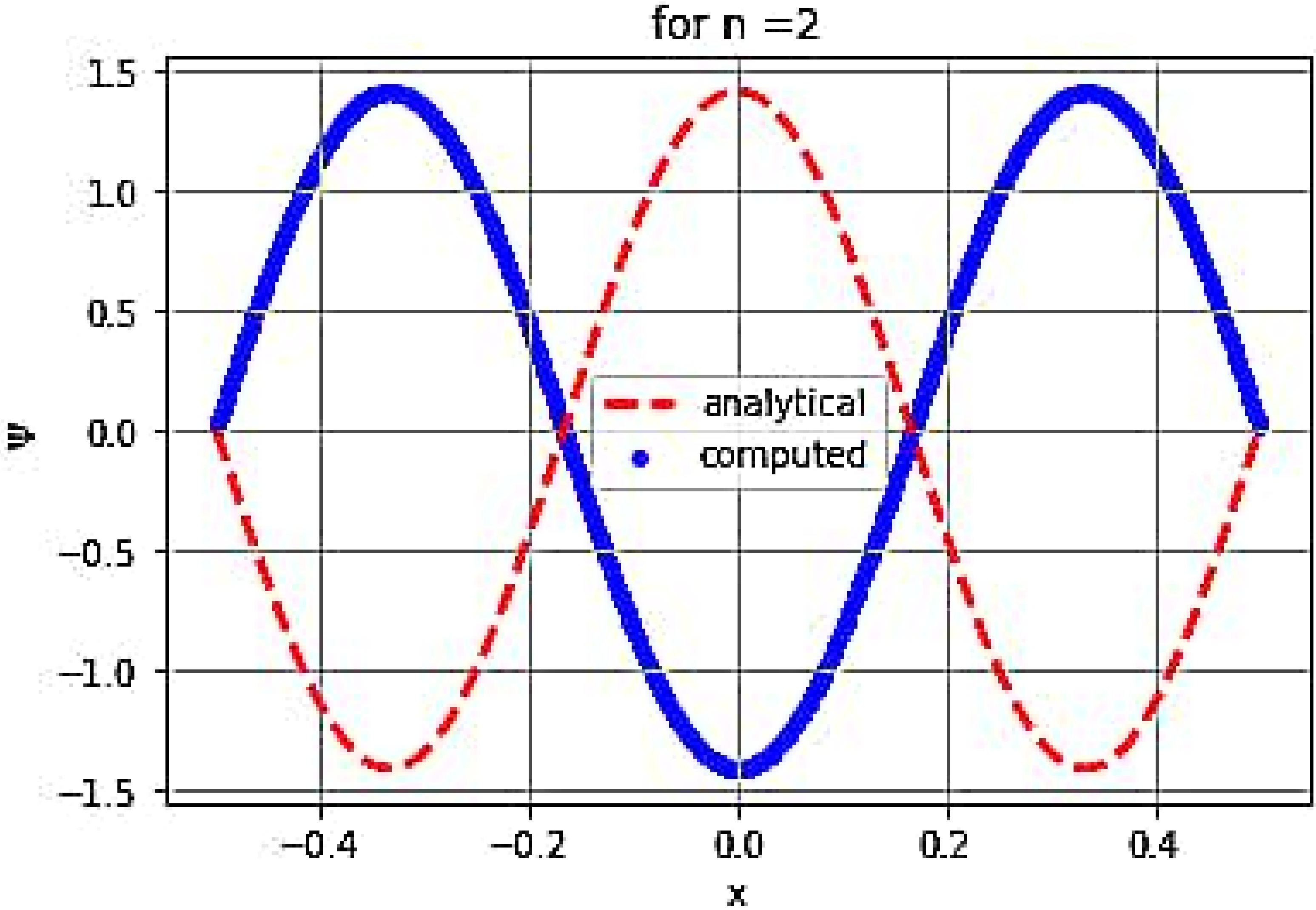
```python

for i in range(4):

    u = sol[1][:, i]
    x  =sol[2]
    norm_u = normalize(x, u)[1]  #normalised wave using normalise function

    U_sq_list.append(norm_u**2)
    if i % 2 != 0 : #odd states

        anal =  np.sin((i+1)*np.pi*x)
        anal_norm = normalize(x, anal)[1]

    else : #even states
        anal =  np.cos((i+1)*np.pi*x)
        anal_norm = normalize(x, anal)[1]

    Anal_U_sq_list.append(anal_norm**2)

    #plot for U vs X

    plots(x, norm_u,anal_norm, ylabel='Ψ', title = "PLOT OF Ψ VS X FOR N= "+str(i),num=1)

#plot for U**2 vs X on the same plot

plots(x, U_sq_list, Anal_U_sq_list, ylabel='Ψ **2', title = "PROBABILITY DENSITY PLOT OF Ψ**2 VS X", num = len(U_sq_list),color = [['r','b'],['y','g'],['m','c'],['k','violet']])
```

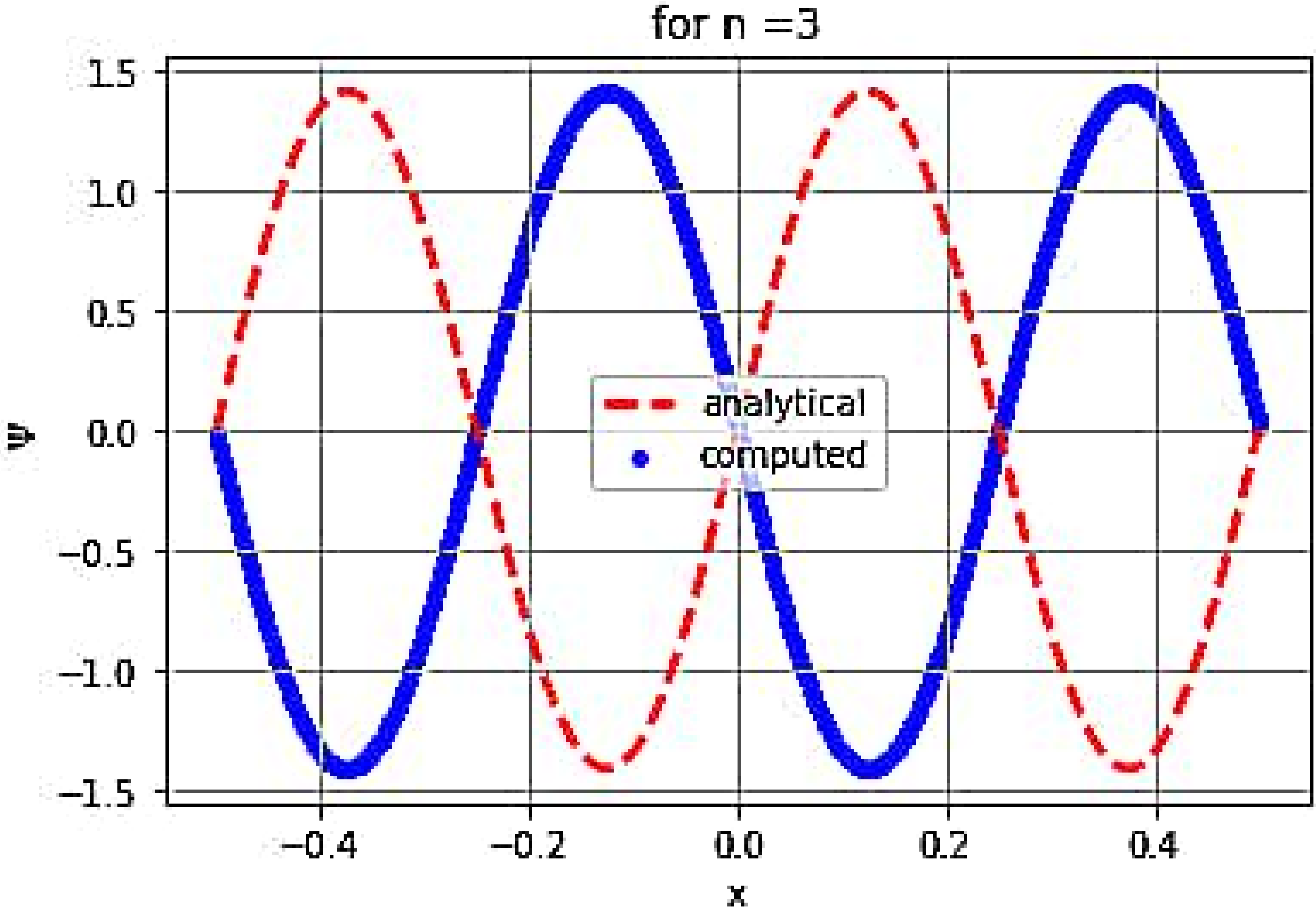
```
In [7]: runfile('D:/python work/prog sem 5/untitled4.py', wdir='D:/python work/prog sem 5')
THE FIRST 10 EIGEN VALUES CALCULATED USING FINITE DIFFERENCE METHOD ARE :
   COMPUTED e  ANALYTICAL e
0    9.830197      9.869604
1   39.320690     39.478418
2   88.471190     88.826440
3  157.281212    157.913670
4  245.750078    246.740110
5  353.876916    355.305758
6  481.660663    483.610616
7  629.100059    631.654682
8  796.193652    799.437956
9  982.939796    986.960440
```

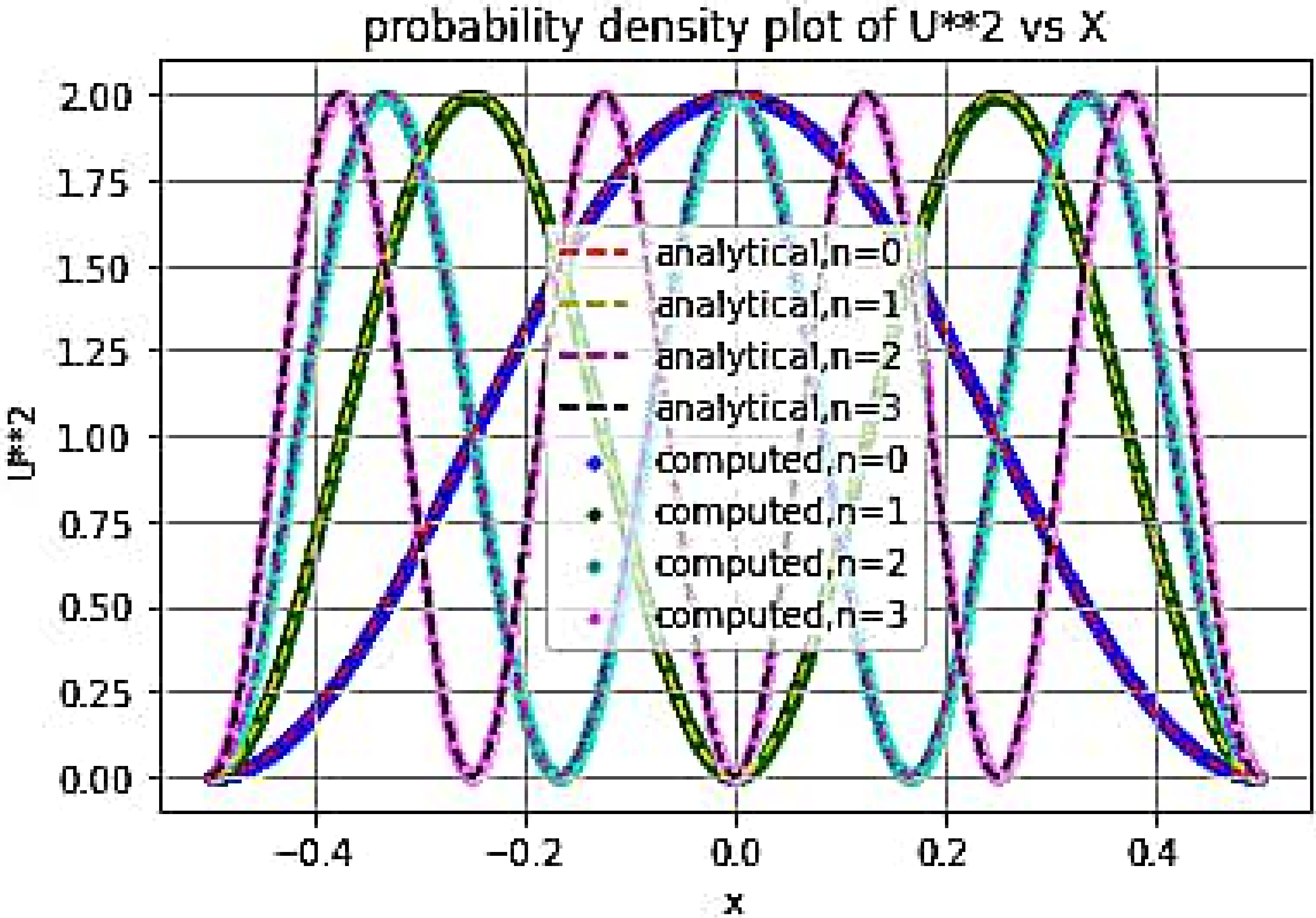


for n =0
analytical
computed
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
ψ
−0.4
−0.2
0.0
0.2
0.4
x


for n =1
analytical
computed
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
ψ
−0.4
−0.2
0.0
0.2
0.4
x


for n =2
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
ψ
analytical
computed
−0.4
−0.2
0.0
0.2
0.4
x


for n =3
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
ψ
analytical
computed
−0.4
−0.2
0.0
0.2
0.4
x


probability density plot of U**2 vs X
2.00
1.75
1.50
1.25
1.00
0.75
0.50
0.25
0.00
U**2
−0.4
−0.2
0.0
0.2
0.4
x
analytical,n=0
analytical,n=1
analytical,n=2
analytical,n=3
computed,n=0
computed,n=1
computed,n=2
computed,n=3

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Q) $H\psi = E\psi$

$$\frac{d^2\psi}{dx^2} = (V+e)\psi$$

$\psi_j'' = (V_j + e)\psi_j$ —① [for any index j]

we also know;

$$\psi_j'' = (\psi_{j+1} + \psi_{j-1} - 2\psi_j)/h^2$$

and $\psi_j'' - V_j\psi_j = e\psi_j$ (from eq①)

~~for j=1~~ so;

$$\frac{1}{h^2}\left[\psi_{j+1} + \psi_{j-1} - 2\psi_j\right] - V_j\psi_j = e\psi_j$$

for $j=1$

$$\frac{1}{h^2}\left[\psi_2 + \psi_0 - 2\psi_1\right] - V_1\psi_1 = e\psi_1$$

$$\frac{1}{h^2}\left[\cancel{\psi_0} - 2\psi_1 + 1\psi_2 + 0\psi_3 + 0\psi_4\right] - V_1\psi_1 = e\psi_1$$

we here ~~take~~ as example for $j=1$ to $j=4$ so,
ψ_j at $j=1$ and $j=4$ i.e boundary point must be zero.

so;
for $j=1$
we have

$$\frac{1}{h^2}\left[-2\psi_1 + 1\times\psi_2 + 0\psi_3 + 0\psi_4\right] - V_1\psi_1 = e\psi_1 \quad \text{—②}$$

for $j=2$

$$\frac{1}{h^2}\left[\vartheta_3+\vartheta_1-2\vartheta_2\right]-V_2\vartheta_2=e\vartheta_2$$

$$\frac{1}{h^2}\left[1.\vartheta_1-2\vartheta_2+1\vartheta_3+0\vartheta_4\right]-V_2\vartheta_2=e\vartheta_2 \quad -③$$

for $j=3$

$$\frac{1}{h^2}\left[\vartheta_4+\vartheta_2-2\vartheta_3\right]-V_3\vartheta_3=e\vartheta_3$$

$$\frac{1}{h^2}\left[0.\vartheta_1+1.\vartheta_2-2\vartheta_3+1.\vartheta_4\right]-V_3\vartheta_3=e\vartheta_3 \quad -④$$

for $j=4$

$$\frac{1}{h^2}\left[\vartheta_5+\vartheta_3-2\vartheta_4\right]-V_4\vartheta_4=e\vartheta_4$$

$$\frac{1}{h^2}\left[0.\vartheta_1+0.\vartheta_2+1\vartheta_3-2\vartheta_4\right]-V_4\vartheta_4=e\vartheta_4 \quad -⑤$$

[$\because \vartheta_5=0$; wave function is zero except in between $j=1$ to 3]

So, On combining eq ②, ③, ④ & ⑤ we get

$$\left[\frac{1}{h^2}\begin{bmatrix}-2 & 1 & 0 & 0\\ 1 & -2 & 1 & 0\\ 0 & 1 & -2 & 1\\ 0 & 0 & 1 & -2\end{bmatrix}-\begin{bmatrix}V_1\\ V_2\\ V_3\\ V_4\end{bmatrix}\right]\vartheta=e\vartheta$$

$$H\vartheta=e\vartheta$$

~~so for any general~~

so, the general formula is :-

$$H = \frac{1}{h^2}\begin{bmatrix} -2 & 1 & 0 & 0 & 0 & \cdots & \cdots \\ 1 & -2 & 1 & 0 & \cdot & 0 & \cdots \\ 0 & 1 & -2 & 1 & 0 & \cdots & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & - & - & - & - & - & \cdot \\ \cdot & - & - & - & - & \cdot & \\ \cdot & - & - & - & \cdots & 1 & -2 \end{bmatrix}_{n \times n} - \begin{bmatrix} V_1 \\ V_2 \\ \cdot \\ \vdots \\ \vdots \\ V_n \end{bmatrix}_{n \times 1}$$

we can use this matrix to find the eigen values and thus eigen functions of the eqn.

+ Discussion :-

1. from the table we can say that; eigen values calculated using finite - difference method is similar to the ones obtained analytically

2. from the plots, we can say that: the eigen functions and probability density obtained using finite difference method and the analytical ones are similar

b) ~~a = a~~

x is in between; $-\frac{a}{2}$ to $\frac{a}{2}$

for dimensionless case:, $z = \frac{x}{a}$

so, z is in range $[-\frac{1}{2}, \frac{1}{2}]$

$n = 3$ (grid points)

so; $h = \frac{b-a}{(n-1)} = \frac{0.5+0.5}{3-1} = \frac{1}{2} = 0.5$

we have; using finite difference method

$$(K+V)\psi = e\psi$$

here,

$$K = \frac{-1}{h^2}\begin{bmatrix} -2 & 1 & 0 \\ 1 & -2 & 1 \\ 0 & 1 & -2 \end{bmatrix}$$

$$V = \begin{bmatrix} V_1 & 0 & 0 \\ 0 & V_2 & 0 \\ 0 & 0 & V_3 \end{bmatrix}$$

for 1-d box case

$V_1, V_2, V_3 = 0$

so;

$$H = K+V = \frac{-1}{h^2}\begin{bmatrix} -2 & 1 & 0 \\ 1 & -2 & 1 \\ 0 & 1 & -2 \end{bmatrix}$$

$$= -4\begin{bmatrix} -2 & 1 & 0 \\ 1 & -2 & 1 \\ 0 & 1 & -2 \end{bmatrix}$$

$$= \begin{bmatrix} 8 & -4 & 0 \\ -4 & 8 & -4 \\ 0 & -4 & 8 \end{bmatrix}$$

To find eigen values and eigen states

$H\vartheta = e\vartheta$

so:

$$|H - eI| = 0$$

$$\begin{vmatrix} 8-e & -4 & 0 \\ -4 & 8-e & -4 \\ 0 & -4 & 8-e \end{vmatrix} = 0$$

$$(8-e)\left[(8-e)^2 - 16\right] - (-4)\left[-4(8-e)\right] = 0$$

$$(8-e)\left[(8-e)^2 - 16\right] - (8-e)(16) = 0$$

$$(8-e)\left[(8-e)^2 - 16 - 16\right] = 0$$

$$(8-e)\left[(8-e)^2 - 32\right] = 0$$

$$(8-e)\left[(8-e-4\sqrt{2})(8-e+4\sqrt{2})\right] = 0$$

$$(8-e)(2.3431-e)(13.6568-e) = 0$$

So, The eigen values are

$e = 2.3431,\ 8$ and 13.6568

The corresponding eigen ~~funct~~ vectors are as

$$\vartheta_1 = [0.5,\ -0.7071,\ -0.5]$$

$$\vartheta_2 = [0.7071,\ 0.1099,\ 0.7071]$$

$$\vartheta_3 = [0.5,\ 0.7071,\ 0.5]$$