# Assignment 2 - Particle in a Box

**SGTB Khalsa College, University of Delhi**

**Preetpal Singh(2020PHY1140)(20068567043)**

**Unique Paper Code: 32221501**

**Paper Title: Quantum Mechanics and Applications**

**Submitted on: August 02, 2022**

**B.Sc(H) Physics Sem V**

**Submitted to: Dr. Mamta**

Preetpal Singh
Roll No. : 2020PHY1140
Subject Quantum Mechanics

Paper Code: 32221501
Assignment 2 (Particle in a Box)

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

Q. Schrodinger Equation for quantum particle of mass m in potential $V(x)$. $\Psi(x,t) = u(x)u(t)$ when potential is independent of time - Determine $f(t)$ & find equation satisfied by function $u(x)$?

Ans Schrodinger Equation for quantum particle of mass m is:

$$i\hbar \frac{d\psi(x,t)}{dt} = -\frac{\hbar^2}{2m}\frac{d^2\psi(x,t)}{dt^2} + V\psi(x,t)$$

Take $\psi(x,t) = u(x) f(t) =$

$$i\hbar\, u(x) \frac{d f(t)}{dt} = f(t)\left[-\frac{\hbar^2}{2m}\frac{d^2 u(x)}{dt} + V \times u(x)\right]$$

$$= f(t) \times \left[-\frac{\hbar^2}{2m}\nabla^2 + V\right] u(x)$$

$$= \underbrace{\frac{i\hbar}{f(t)} \frac{df(t)}{dt}}_{t \text{ dependent}} = \underbrace{\frac{1}{u(x)}\left[-\frac{\hbar^2}{2m}\nabla^2 + V\right] u(x)}_{x \text{ dependent}}$$

Let both be equal to constant E

$$i\hbar \frac{d f(t)}{dt} = E f(t) \qquad -(1)$$

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V\right] u(x) = E\, u(x)$$

Integrating (1) gives

$$f(t) = e^{-iEt/\hbar}$$

$$i\hbar \times u(x) \frac{d}{dt} e^{-iEt/\hbar} = e^{-iEt/\hbar}\left[-\frac{\hbar^2}{2m}\nabla^2 + V\right] u(x)$$

$$i\cancel{\hbar} \times u(x) \times e^{-iEt/\hbar} \times \frac{-iE}{\cancel{\hbar}} = e^{-iEt/\hbar}\left[-\frac{\hbar^2\nabla^2}{2m} + V\right] u(x)$$

$$= E u(x)\, e^{-iEt/\hbar} - e^{-iEt/\hbar}\left[-\frac{\hbar^2\nabla^2}{2m} + V\right] u(x) = 0$$

$$e^{-iEt/\hbar}\left[\frac{\hbar^2\nabla^2}{2m} + u(x)\left(E-V\right)\right] = 0$$

Q-2. If $V(x)$ is even function of $x$, show that solution of TISE Schrodinger Equation can be taken to be either even or odd functions.

Ans. If $V(x)$ is even function of $x$, then

$$V(-x) = V(x)$$

Time independent Schrodinger wave equation is

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} + V(x)\psi(x) = E\psi(x)$$

Replace $x \to -x$

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(-x)}{\partial x^2} + V(-x)\psi(-x) = E\psi(-x)$$

Now, There are 2 cases

Case 1: If eigen value is non degenerate then $\psi(x)$ and $\psi(-x)$ differ by multiplicative constant

$$\psi(-x) = c\psi(x)$$

$$\psi(x) = c\psi(-x) \Rightarrow \psi(x) = c^2\psi(x)$$

$$c^2 = 1$$

$$c = \pm 1$$

$$\psi(-x) = \pm\psi(x)$$

Case 2: If eigen value is degenerate, then $\psi(x)$ & $\psi(-x)$ are two linearly independent solutions

$$\psi_+(x) = \psi(x) + \psi(-x)$$

$$\psi_-(x) = \psi(x) - \psi(-x)$$

(c) Solve Schrodinger Equation for a particle in a 1-d box analytically in the range $\left[-\frac{L}{2} : \frac{L}{2}\right]$ ie.

$$V(x) = \begin{cases} 0 & \text{for } |x| < L/2 \\ \infty & \text{otherwise} \end{cases}$$

Ans $\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} E\psi = 0$ Take $k = \sqrt{\frac{2mE}{\hbar^2}}$ $\Rightarrow$ $\frac{d^2\psi}{dx^2} + k^2\psi = 0$

The solution of schrodinger wave eqn for 1-d box is

$$\psi(x) = A\cos(kx) + B\sin(kx)$$

For this $\psi(x)$ to be solution of schrodinger wave equation, it must satisfy the boundary conditions at $x = -L/2$ and $x = \frac{L}{2}$

(i) At $x = \frac{L}{2}$, $\psi(x) = \psi\left(\frac{L}{2}\right) = 0$

$$\psi\left(\frac{L}{2}\right) = A\cos\left(\frac{kL}{2}\right) + B\sin\left(\frac{kL}{2}\right) = 0$$

To make this equation ~~equal~~ equals to zero, then either $A\cos\left(\frac{kL}{2}\right) = 0$ or $B\sin\left(\frac{kL}{2}\right) = 0$

As $\sin\left(\frac{kL}{2}\right)$ and $\cos\left(\frac{kL}{2}\right)$ are oscillatory functions, so they can't be equal to zero for all values of $x$.

if $A = 0$

$$\cancel{\cos}\; B\sin\left(\frac{kL}{2}\right) = 0$$

$$\frac{kL}{2} = n\pi$$

$$k = \frac{2n\pi}{L}, \text{ for } n = 1, 2, ----$$

$$\psi_1 = B\sin\left(\frac{2n\pi}{L} x\, x\right)$$

if $B = 0$

$$A\cos\left(\frac{kL}{2}\right) = 0$$

$$\frac{kL}{2} = \frac{(2n+1)\pi}{2}$$

$$k = \frac{(2n+1)\pi}{L}$$

$$\psi_2 = A\cos\left(\frac{(2n+1)\pi}{L}x\right)$$

Now, to determine the constants A and B, Normalising the wavefunction

$$\int_{-\infty}^{\infty} |\psi|^2 dx = 1 \quad \Rightarrow \int_{-L/2}^{L/2} |\psi|^2 dx = 1$$

$\Rightarrow$ For $\psi_1 = B\sin\left(\frac{2n\pi}{L}x\right)$

$$B^2 \int_{-L/2}^{L/2} \sin^2\left(\frac{2n\pi}{L}x\right) dx = 1$$

$$\frac{B^2}{2} \int_{-L/2}^{L/2} \left(1 - \cos\left(\frac{4n\pi}{L}x\right)\right) dx = 1 \qquad \cos 2x = 1 - 2\sin^2 x$$

$$\sin^2 x = \frac{1-\cos 2x}{2}$$

$$\frac{B^2}{2}\left[x - \frac{\sin\left(\frac{4n\pi}{L}x\right)}{\frac{4n\pi}{L}}\right]_{-L/2}^{L/2} = 1$$

$$= \frac{B^2}{2}\left[\left(\frac{L}{2} - \frac{\sin\left(\frac{4n\pi}{L}\times\frac{L}{2}\right)}{\frac{4n\pi}{L}}\right) - \left(\frac{-L}{2} - \frac{\sin\left(\frac{4n\pi}{L}\times\frac{-L}{2}\right)}{\frac{4n\pi}{L}}\right)\right]$$

$$= \frac{B^2}{2}\left[L\right] = 1$$

$$B^2 = \frac{2}{L}$$

$$\boxed{B = \sqrt{\frac{2}{L}}}$$

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

$$\int_{-L/2}^{L/2} |\psi_2|^2 dx = \frac{1}{2}A^2 \int_{-L/2}^{L/2} \cos\left(2\times\left(\frac{(2n+1)\pi x}{L}\right)\right) dx + \int_{-L/2}^{L/2} 1\, dx$$

$\cos 2x = 2\cos^2 x - 1$

$\cancel{\cos 2}\ \cos^2 x = \frac{\cos 2x + 1}{2}$

$$A^2 \frac{1}{2}\left[\left[\left(\frac{-\sin\left(\frac{2\times(2n+1)\pi}{\cancel{L}}\times\frac{\cancel{L}}{2}\right)}{\frac{2(2n+1)\pi}{L}} + \frac{L}{2}\right) - \left(\frac{-\sin\left(\frac{2(2n+1)\pi}{\cancel{L}}\times\frac{-\cancel{L}}{2}\right)}{\frac{2(2n+1)\pi}{L}} - \frac{L}{2}\right)\right]\right] = 1$$

$$A^2 \frac{1}{2}\times L = 1$$

$$\boxed{A = \sqrt{\frac{2}{L}}}$$

$$\psi(x) = \psi_1(x) + \psi_2(x)$$

$$\boxed{\psi(x) = \sqrt{\frac{2}{L}}\left[\sin\left(\frac{2n\pi x}{L}\right) + \cos\left(\frac{(2n+1)\pi x}{L}\right)\right]}$$

(d) Convert Schrodinger Equation for infinite potential well into dimensionless form and write down the energy eigen values in dimensionless form(e). obtain energy E in physical units from numerical soln into dimensionless form.

Ans. Schrodinger Equation for infinite potential well

$$\frac{d^2\psi}{dx^2} + \frac{2mE}{\hbar^2}\psi = 0 \quad -(1)$$

Take $\; x_1 = \frac{x}{L}$

$$\frac{dx_1}{dx} = \frac{1}{L}$$

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

$$\frac{d\psi}{dx} = \frac{d\psi}{d\xi} \times \frac{d\xi}{dx} = \frac{d\psi}{d\xi} \times \frac{1}{L}$$

$$\frac{d^2\psi}{dx^2} = \frac{d}{dx}\left(\frac{d\psi}{d\xi} \times \frac{1}{L}\right) = \frac{1}{L} \times \frac{d^2\psi}{dx\,d\xi} + \frac{d\psi}{d\xi} \times \underbrace{\frac{d}{dx}\frac{1}{L}}_{0}$$

$$\frac{d^2\psi}{dx^2} = \frac{1}{L}\frac{d^2\psi}{dx\,d\xi} = \frac{1}{L} \times \frac{d}{d\xi}\left(\frac{d\psi}{dx}\right) = \frac{1}{L}\left(\frac{d}{d\xi}\left(\frac{d\psi}{d\xi}\,\frac{d\xi}{dx}\right)\right)$$

$$\frac{d^2\psi}{dx^2} = \frac{1}{L}\left(\frac{d}{d\xi}\left(\frac{d\psi}{d\xi}\,\frac{1}{L}\right)\right)$$

$$\frac{d^2\psi}{dx^2} = \frac{1}{L^2}\,\frac{d^2\psi}{d\xi^2}$$

putting value of $\frac{d^2\psi}{dx^2}$ in (1)

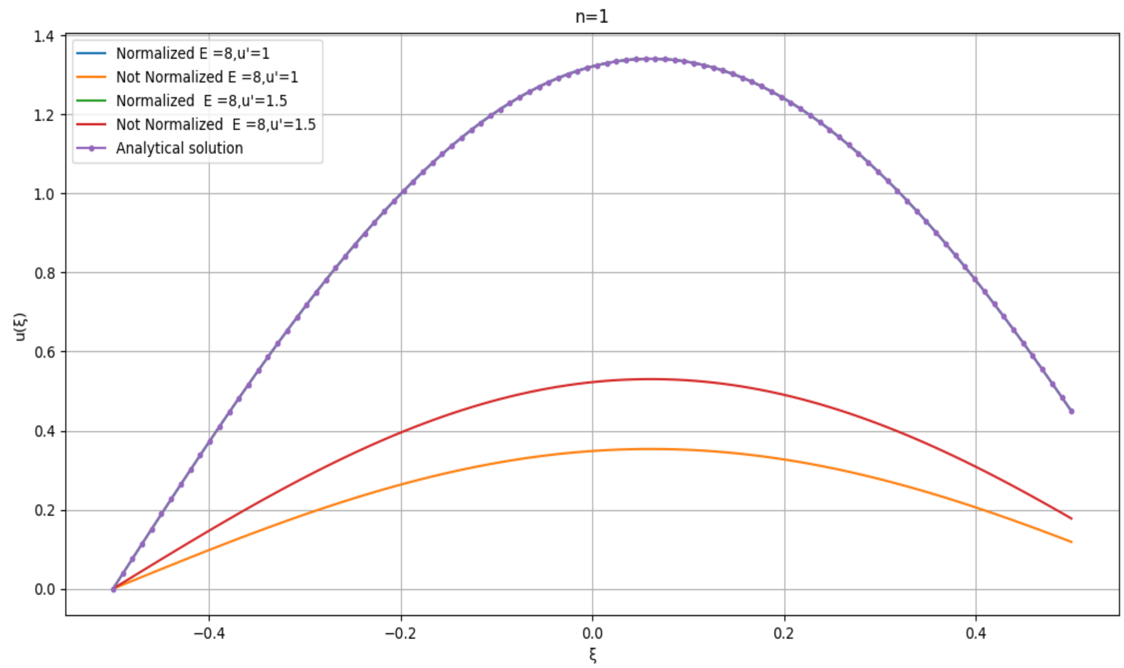
$$\frac{1}{L^2}\frac{d^2\psi}{d\xi^2} + \frac{2mE}{\hbar^2}\psi = 0$$

# Programming

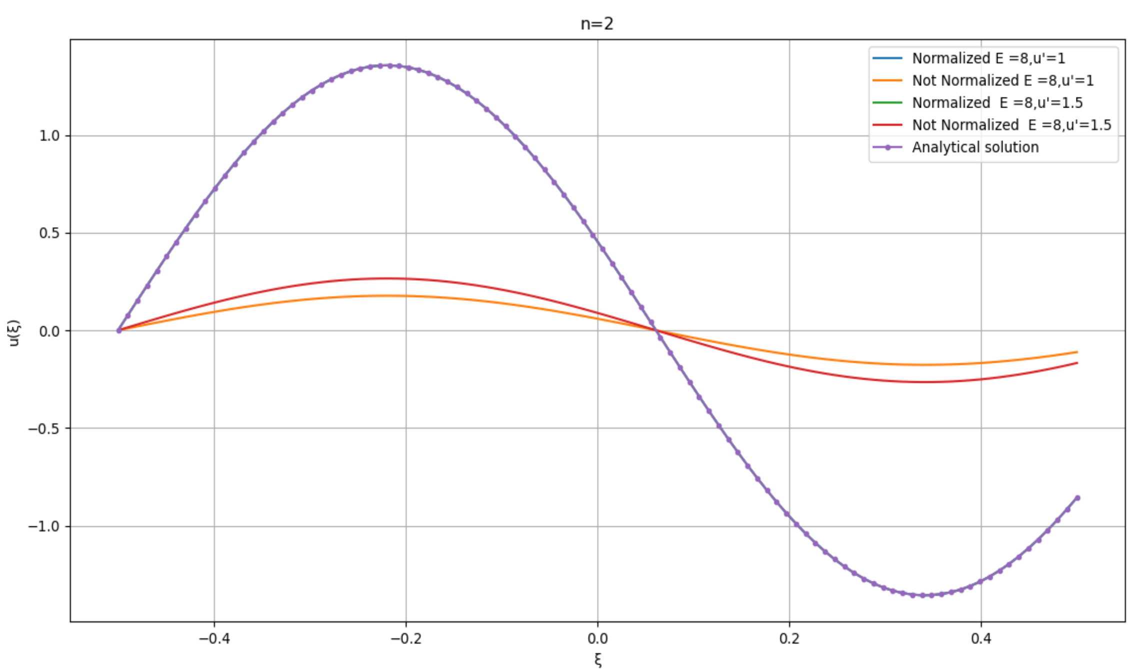
```python
import numpy as np
import matplotlib.pyplot as plt
import pandas as pd
import scipy.integrate as integrate

def My_RK4(Y0,func,xi,xf,n):
    x = np.linspace(xi,xf,n)
    h = (xf-xi)/n
    Y = np.zeros((n,len(Y0)))
    Y[0,:] = Y0
    for i in range(n-1):
        k1 = h*func(x[i],Y[i,:])
        k2 = h*func(x[i]+h*0.5,Y[i,:]+k1*0.5)
        k3 = h*func(x[i]+h*0.5,Y[i,:]+k2*0.5)
        k4 = h*func(x[i]+h,Y[i,:]+k3)
        Y[i+1,:] = Y[i,:]+(k1+2*k2+2*k3+k4)/6
    return Y

def func_(x,x_vec):
    ans_vec = np.zeros((2))
    ans_vec[0] = x_vec[1]
    ans_vec[1] = (-n**2)*(8)*x_vec[0]
    return ans_vec

def analytical(x,n):
    u_ana = []
    for i in range(n):
        if (i%2)== 0:
            u = np.sqrt(2)*np.cos(n*np.pi*x)
            u_ana.append(u)
        else:
            u = np.sqrt(2)*np.sin(n*np.pi*x)
            u_ana.append(u)
    return u

x  = np.linspace(-1/2,1/2,100)
for n in range(1,5):
    y1  = My_RK4([0,1],func_,0,1,100).T[0]
    y2  = My_RK4([0,1],func_,0,1,100).T[1]
    #normalized
    y=y1/np.sqrt(integrate.simps(y1**2,x))
    plt.rcParams["figure.figsize"] = (15,10)
    plt.plot(x,y,label ="Normalized E =8,u'=1 ")
    plt.plot(x,y1,label ="Not Normalized E =8,u'=1 ")

    y1  = My_RK4([0,1.5],func_,0,1,100).T[0]
    y2  = My_RK4([0,1.5],func_,0,1,100).T[1]
    #normalized
    y=y1/np.sqrt(integrate.simps(y1**2,x))
    plt.rcParams["figure.figsize"] = (15,10)
    plt.plot(x,y,label = "Normalized  E =8,u'=1.5")
    plt.plot(x,y1,label = "Not Normalized  E =8,u'=1.5")

    #Analytical solution
    u = analytical(x,n)
    plt.plot(x,y,marker = ".",label = "Analytical solution")
    plt.title(n)
    plt.grid()
    plt.legend()
    plt.show()

def func_(x,x_vec):
    ans_vec = np.zeros((2))
    ans_vec[0] = x_vec[1]
    ans_vec[1] = (-n**2)*(11)*x_vec[0]
```

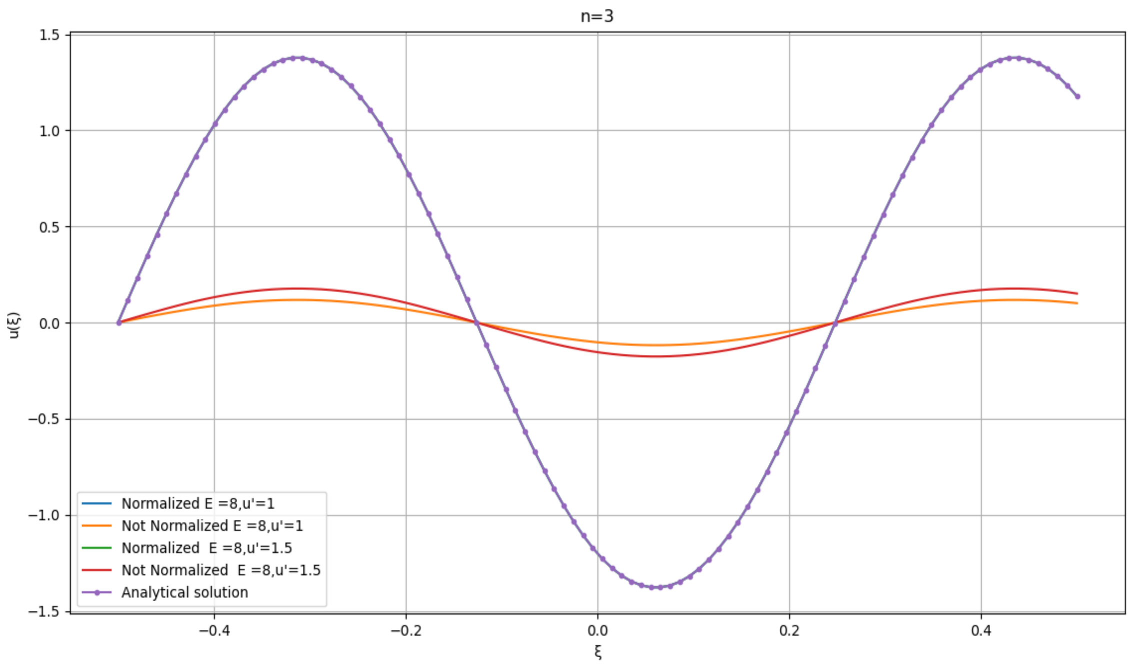
```python
    return ans_vec

def analytical(x,n):
    u_ana = []
    for i in range(n):
        if (i%2)== 0:
            u = np.sqrt(2)*np.cos(n*np.pi*x)
            u_ana.append(u)
        else:
            u = np.sqrt(2)*np.sin(n*np.pi*x)
            u_ana.append(u)
    return u

x  = np.linspace(-1/2,1/2,100)

for n in range(1,5):
    y1  = My_RK4([0,1],func_,0,1,100).T[0]
    y2  = My_RK4([0,1],func_,0,1,100).T[1]
    #normalized
    y=y1/np.sqrt(integrate.simps(y1**2,x))
    plt.rcParams["figure.figsize"] = (15,10)
    plt.plot(x,y,label ="Normalized E =11,u'=1 ")
    plt.plot(x,y1,label ="Not Normalized E =11,u'=1 ")

    y1  = My_RK4([0,1.5],func_,0,1,100).T[0]
    y2  = My_RK4([0,1.5],func_,0,1,100).T[1]
    #normalized
    y=y1/np.sqrt(integrate.simps(y1**2,x))
    plt.rcParams["figure.figsize"] = (15,10)
    plt.plot(x,y,label ="Normalized E =11,u'=1 ")
    plt.plot(x,y1,label ="Not Normalized E =11,u'=1 ")

    #Analytical solution
    u = analytical(x,n)
    plt.plot(x,y,marker = ".",label = "Analytical solution")
    plt.grid()
    plt.title(n)
    plt.legend()
    plt.show()


def func_(x,x_vec):
    ans_vec = np.zeros((2))
    ans_vec[0] = x_vec[1]
    ans_vec[1] = (-n**2)*(E**2)*x_vec[0]
    return ans_vec

x  = np.linspace(-1/2,1/2,100)
epsilonvalue = np.linspace(np.pi*0.9,1.1*np.pi,10)

for n in range(1,5):
    for i in range(len(epsilonvalue)):
        E = epsilonvalue[i]
        y1  = My_RK4([0,1],func_,0,1,100).T[0]
        y2  = My_RK4([0,1],func_,0,1,100).T[1]
        plt.rcParams["figure.figsize"] = (15,10)
        plt.plot(x,y1,label = epsilonvalue[i]**2)
    plt.grid()
    plt.legend()
    plt.show()
```

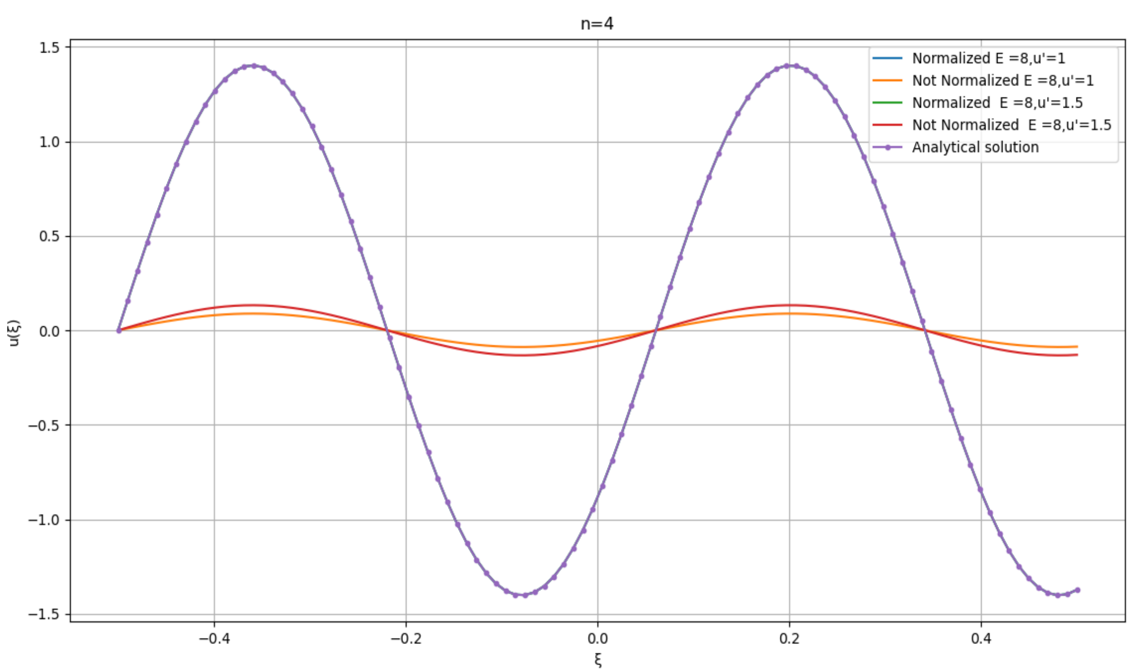
# Result and Discussion

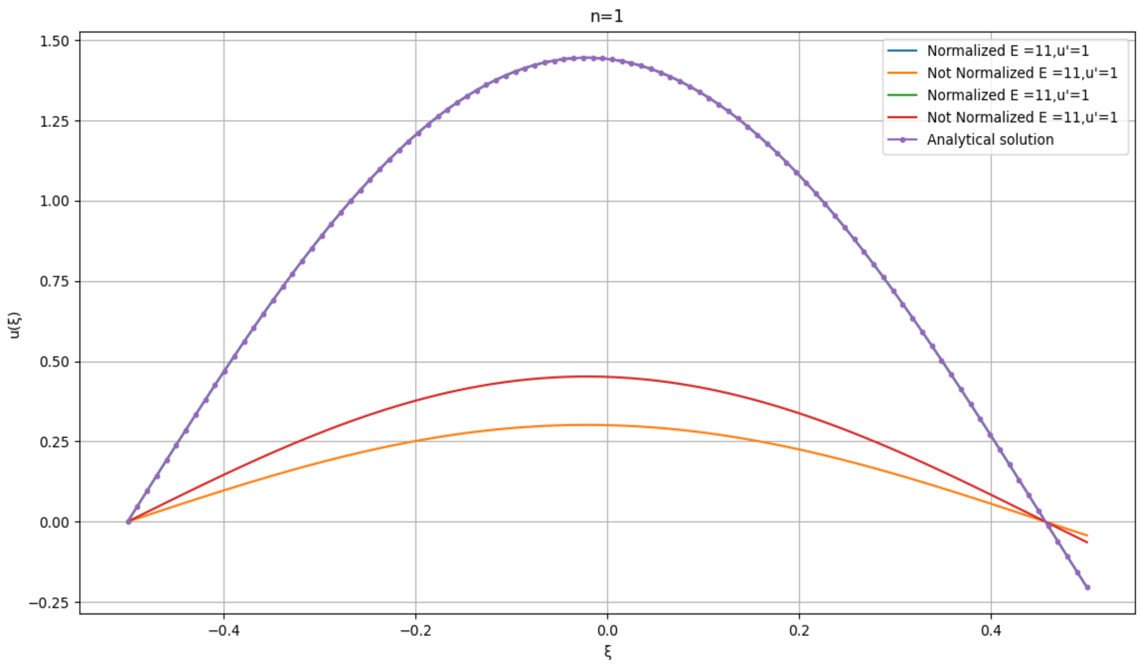


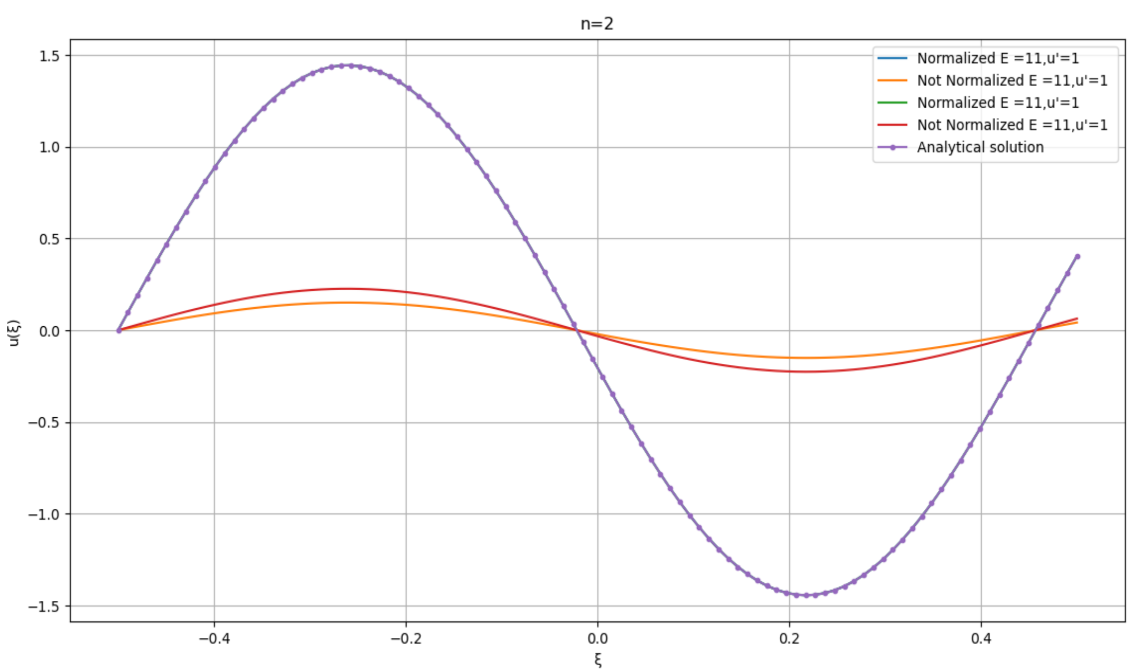

The given figure shows

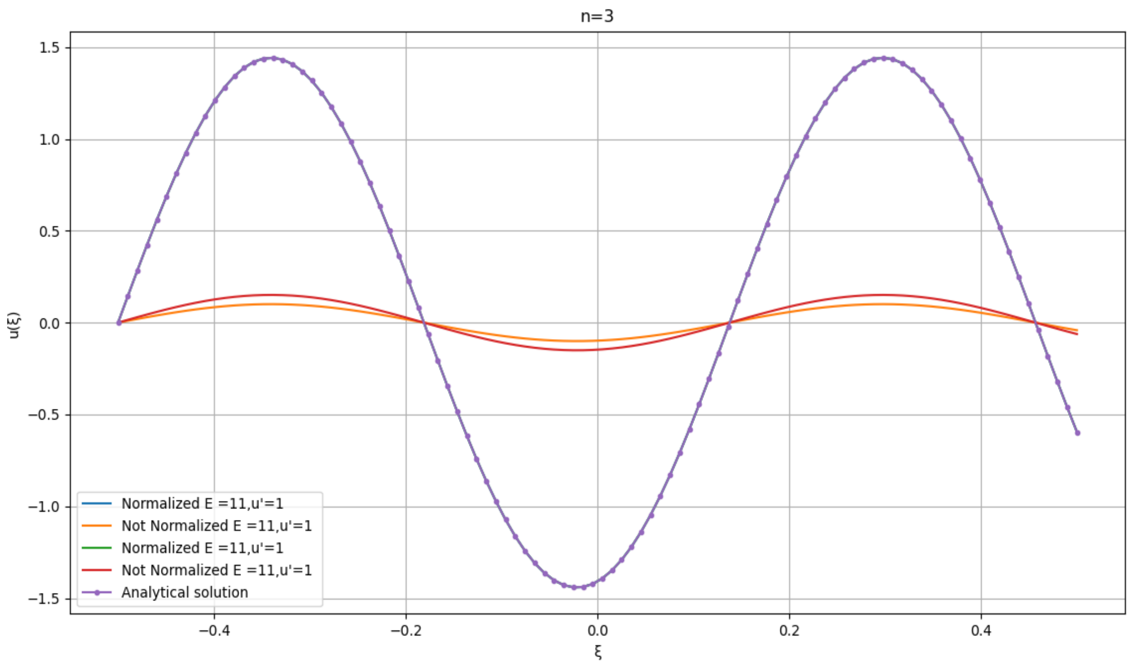


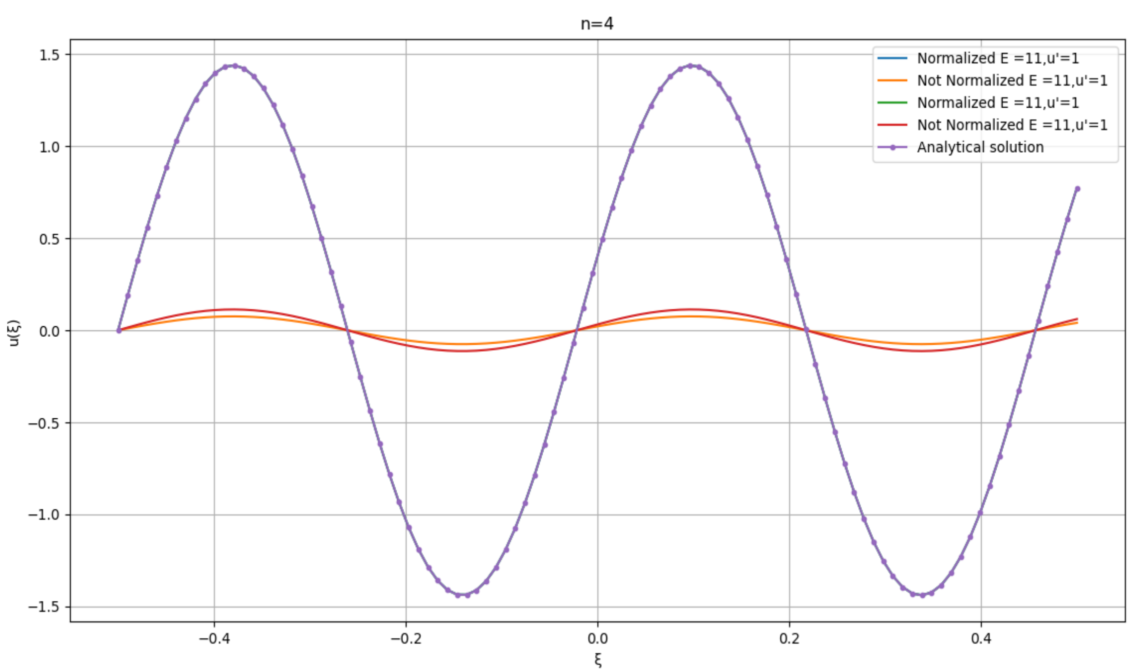

n=3
u(ξ)
ξ
Normalized E =8,u'=1
Not Normalized E =8,u'=1
Normalized E =8,u'=1.5
Not Normalized E =8,u'=1.5
Analytical solution

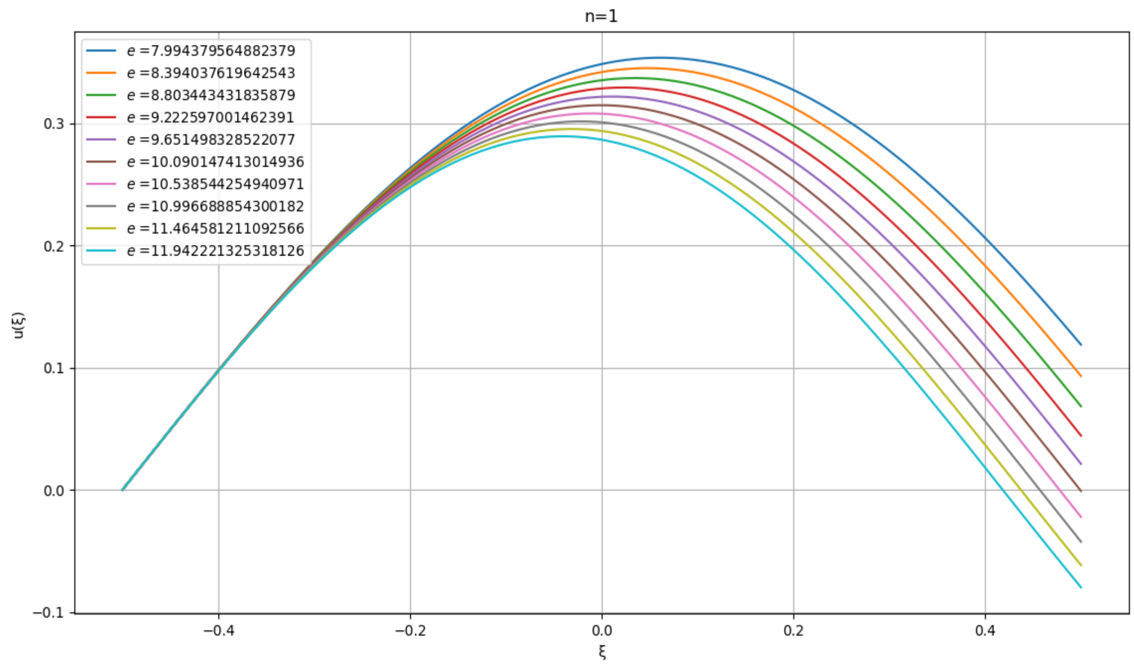

n=4
u(ξ)
ξ
Normalized E =8,u'=1
Not Normalized E =8,u'=1
Normalized E =8,u'=1.5
Not Normalized E =8,u'=1.5
Analytical solution

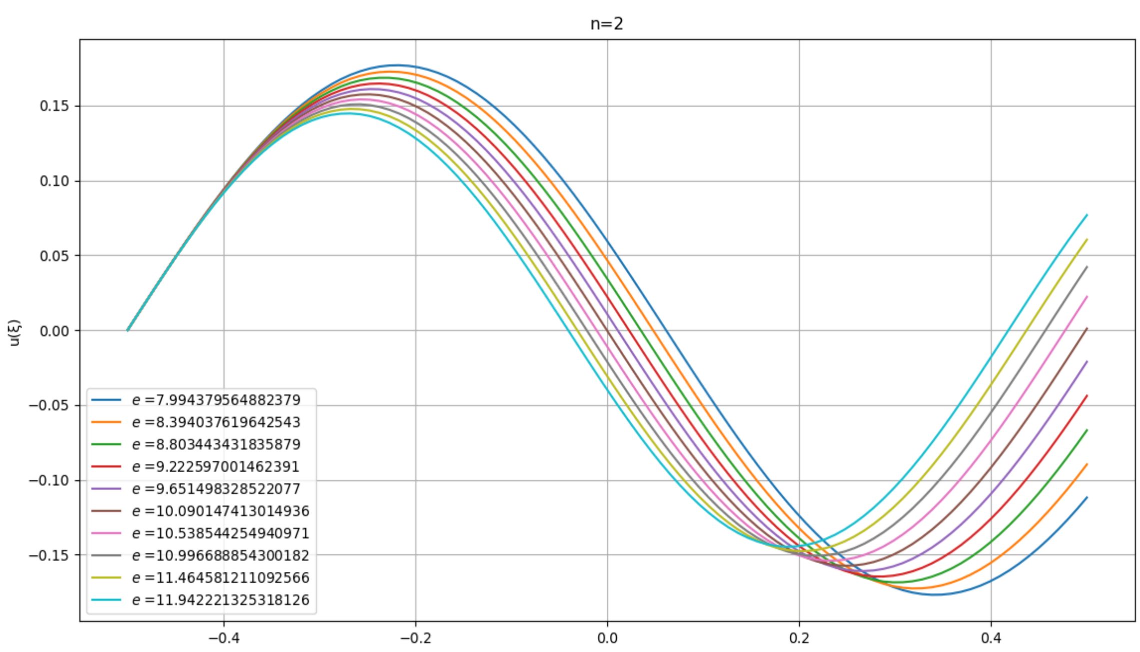

n=1
Normalized E =11,u'=1
Not Normalized E =11,u'=1
Normalized E =11,u'=1
Not Normalized E =11,u'=1
Analytical solution
u(ξ)
ξ

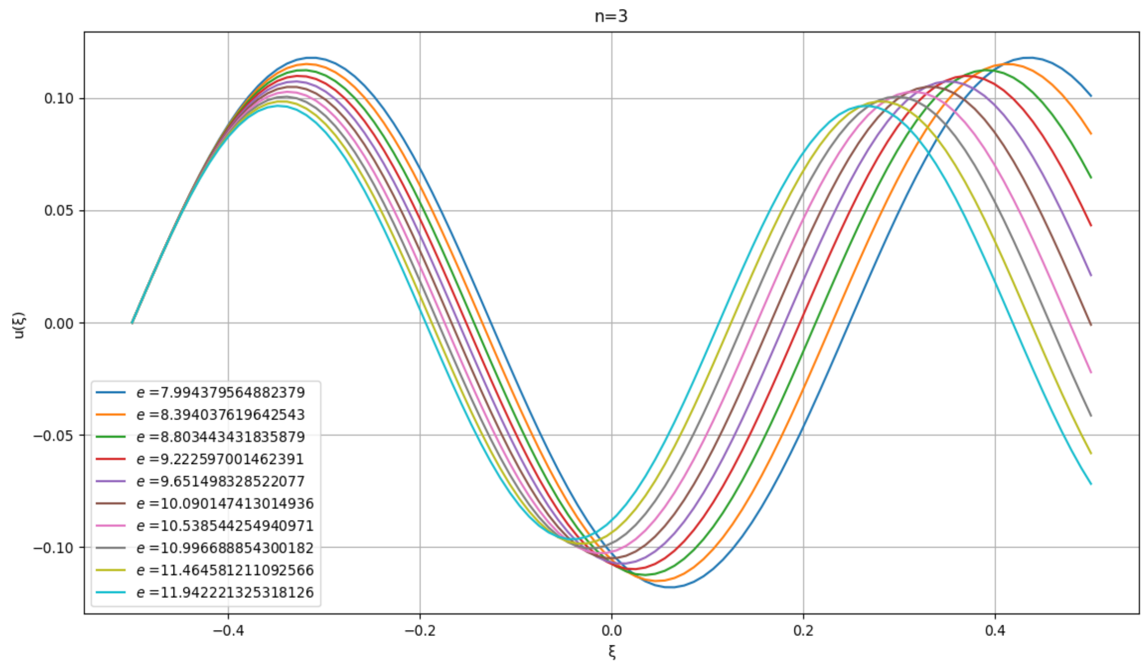

n=2
Normalized E =11,u'=1
Not Normalized E =11,u'=1
Normalized E =11,u'=1
Not Normalized E =11,u'=1
Analytical solution
u(ξ)
ξ

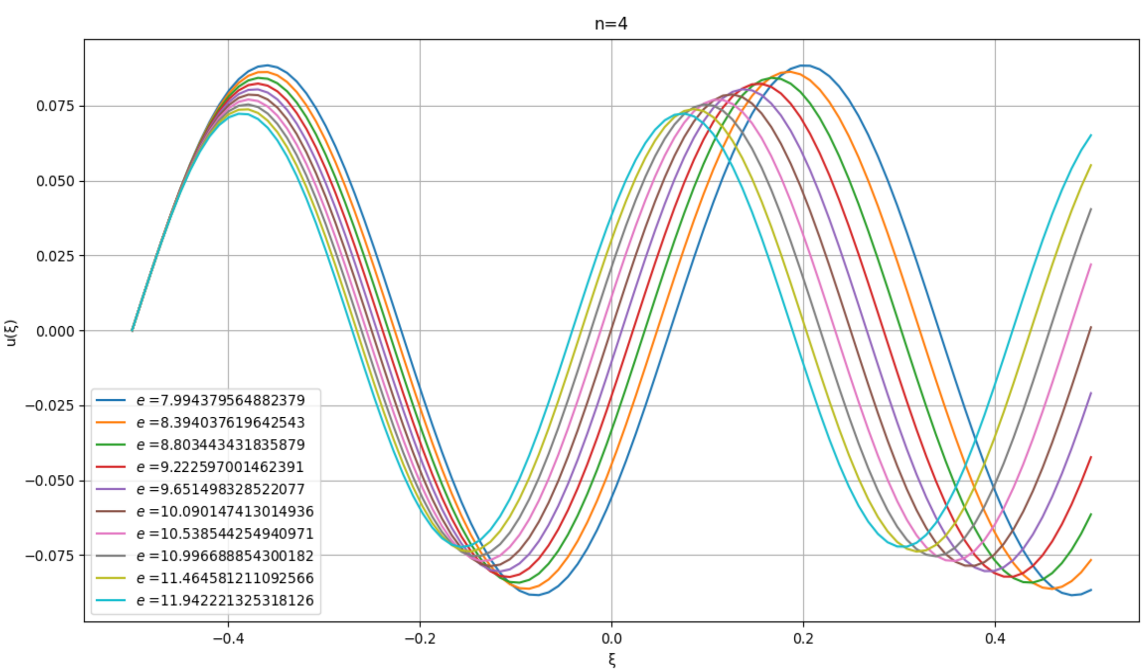

n=3
Normalized E =11,u'=1
Not Normalized E =11,u'=1
Normalized E =11,u'=1
Not Normalized E =11,u'=1
Analytical solution
u(ξ)
ξ


n=4
Normalized E =11,u'=1
Not Normalized E =11,u'=1
Normalized E =11,u'=1
Not Normalized E =11,u'=1
Analytical solution
u(ξ)
ξ


n=1
$e$ =7.994379564882379
$e$ =8.394037619642543
$e$ =8.803443431835879
$e$ =9.222597001462391
$e$ =9.651498328522077
$e$ =10.090147413014936
$e$ =10.538544254940971
$e$ =10.996688854300182
$e$ =11.464581211092566
$e$ =11.942221325318126
u(ξ)
ξ


n=2
$e$ =7.994379564882379
$e$ =8.394037619642543
$e$ =8.803443431835879
$e$ =9.222597001462391
$e$ =9.651498328522077
$e$ =10.090147413014936
$e$ =10.538544254940971
$e$ =10.996688854300182
$e$ =11.464581211092566
$e$ =11.942221325318126
u(ξ)
ξ


n=3
u(ξ)
ξ
e =7.994379564882379
e =8.394037619642543
e =8.803443431835879
e =9.222597001462391
e =9.651498328522077
e =10.090147413014936
e =10.538544254940971
e =10.996688854300182
e =11.464581211092566
e =11.942221325318126


n=4
u(ξ)
ξ
e =7.994379564882379
e =8.394037619642543
e =8.803443431835879
e =9.222597001462391
e =9.651498328522077
e =10.090147413014936
e =10.538544254940971
e =10.996688854300182
e =11.464581211092566
e =11.942221325318126