Assignment 2 - Particle in a Box - II

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Namer Preetpal Singh Assignment Particle in a Box -II					
Roll No. => 2020 PHY1140	Dater August 08, 2022				
Subject + Quantum Mechanics (Rab)	Date/				
1.(a) Particle of mass in trapped in infinite potential well					
V(n)=/0 for In/c 4/2					
The solution of schnodinger were equation in 1-D box for given boundary condition ist					
$\psi(n) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \sin\left(\frac{\partial n}{\partial n}\right) x + 2n$	$ex((2n+1) \sqcap k)$				
For particle in ground state, n=0, 4(n) becomes 4(n) = 2 cm (2nx1) n n T					
P= Jyy dn = Z Cos Lyy - Lyy					
$\begin{array}{c c} & & & & & & \\ & & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\$	$\frac{dn}{cs^2n} = \frac{2cs^2n-1}{2}$				
P= 1 [sin (2 x(2n+1) Hx) / 1	n l				
-4/4 2 (2n+1)11 -1/4					
Y-2 [25in (3x (3nx1) H x !) 1 2 (2nx1) If 2 (2nx1) If	+ 4				
	Spiral				

To make integration easy, writing the and to in below form

y= 12 cos nox noli3151 ---4= 2 SINNTE h=214,---My is real, a 4- 4x
To calculate in For even state 1/2 1 x > z | 1/2 y x y* dn = | y² n dn -1/2 -1/2 2) 215in2 niTR dox = 0 For odd state LA) 2 Janx cos2 mm dre = 6 . (n7=0 for n=1,2,3, ---

To tind Cx2> $\angle \hat{n}^2 > = 2 \int n^2 \sin^2 ni x \, dx$ Colluc 1-25122 = 1 1 x2 (1- cos 2x nnx) dx = 1 July - July 200 2011x du $\frac{1}{2}\left[\frac{n^3}{3}\right]^{2/2} - \left[\frac{4n^2n^2}{2}\right]^2 - 2\sin \frac{2n\pi x}{2} + 2n\pi x + 2n\pi x$ $\frac{2 \sqrt{1 + 23}}{2 \sqrt{3}} = \frac{2 \sqrt{3}}{2 \sqrt{3}} =$ $-\frac{1}{L}\begin{bmatrix} L^{3} & L^{3} \\ 12 & 2h^{2}\Pi^{2} \end{bmatrix} - \begin{bmatrix} L^{2} & 2^{2} \\ 12 & 2h^{2}\Pi^{2} \end{bmatrix}$

$$\angle \hat{\chi}^2 > = \begin{bmatrix} L^2 - \frac{L^2}{2n^2\Pi^2} \end{bmatrix}$$
 for $y_1 = 2 \cdot 1 \cdot 1 \cdot 1 \cdot 6 \cdot - - -$

$$2x^{2} = \int_{-1/2}^{1/2} \psi^{2} n^{2} dn - 2 \int_{-1/2}^{1/2} n^{2} \cos^{2} n n x$$

$$\frac{1}{2} \frac{1}{2} \frac{1}$$

$$-\frac{1}{2} \left[\frac{(x^3)^{\frac{1}{2}}}{3} + \left[\frac{(y_n)^2 \pi^2 x^2}{L^2} - 2 \right] \sin 2 \pi \pi x + \frac{(y_n)^2 \pi^2 x^2}{L} + \frac{(y_n)^2 x^2}{L} + \frac{(y_n)^2$$

$$= \frac{1}{2} \left[\frac{1^{3}}{1^{2}} - \frac{1^{3}}{2h^{2}} \right]^{\frac{1}{2}}$$

$$\frac{\Lambda^2}{\langle \lambda^2 \rangle} = \frac{L^2}{1e} - \frac{L^2}{2h^2 n^2}$$

So
$$(\frac{2}{2})^2 = \frac{1^2}{12} + \frac{1^2}{2n^2 \cdot 1^2} + \frac{1}{2} \cdot \frac{1$$

$$5x = \frac{L^2}{12} - \frac{L^2}{2n^2 \Pi^2}$$

For unamentan, $\beta = -ik \frac{2}{2x}$
1/2 1/2 1/2 1/2 1/2 1/2 1/2 1/2 1/2 1/2
$\frac{2}{\sqrt{2}} = \int_{-1/2}^{1/2} \psi \int_{-1/2}$
-1/2 -1/2
As 4 is real, so 4=4*
He
= J4 (-it 24) dx
-1/2
For even State
1 100 1 F3 (F3 (F3) 1)
$\frac{1}{2} = \frac{1}{2} \int_{-\frac{1}{2}}^{2} \frac{1}{2} \sin \frac{\pi}{2} \times \frac{1}{2} \int_{-\frac{1}{2}}^{2} \frac{1}{2} \sin \frac{\pi}{2} dx$
It 12 Sin h TIX X Cos h 17x x n 17 doc
1,
1 & x 2 hir Sin hira Cos hrix da = 0
$= -1 \pm x + 2 + 17 = -1 \pm x + 2 = 0$ $= -1 \pm x + 2 + 17 = 0$ $= -1 \pm x + 2 + 17 = 0$
Dr Hagonal
For odd state
2/2
(P) = J = Los nnx x-it = 1 Coo hnx dox
-1/2
412
axtitix htt col hour Sin hour dx =0
1 the way
2 xtit x htt cos nox sin non dx =0 1 Ly Vyord

Spiral

$$\int_{1/2}^{1/2} \int_{1/2}^{1/2} \frac{1}{\sqrt{1+1}} \int_{1$$

For Even State $\angle \beta^2 > = \int \frac{1}{\sqrt{2}} \frac{1}{\sqrt{2}} \frac{1}{\sqrt{2}} \frac{1}{\sqrt{2}} \left(-\frac{1}{\sqrt{2}} \frac{1}{\sqrt{2}} \right) dn$ $\frac{1}{L^{2}} \times \frac{1}{L^{2}} \times \frac{1}{L} \int \frac{\sin^{2} n \pi x}{L} dx$ $\frac{\mathcal{L}^2 n^2 r l^2}{\mathcal{L}^3} \left[\mathcal{A} - \sin \frac{2 n l x}{\mathcal{L}} \right]$ $=\frac{\ell^{2}n^{2}n^{2}}{18}\times\frac{\ell^{2}n^{2}n^{2}}{L^{2}}$ $\angle p^2 = \frac{k^2 n^2 n^2}{L^2}$ $\angle p^2 > = \frac{R^2 n^2 r_1^2}{L^2}$ for n = 1, 2, 3, 12 ((p2) - (p)2)

Sperol

(M) Uncertainty Principle in Dimension less forms Uncertainty principle relation is DPx Dx > t (1) Let's take DP'n and Dn' are in dimensionless forms We can write DPx and Dx' as $DP'_{x} = \frac{DP_{x}}{P} - (2) \qquad Dx' = \frac{Dx}{L} - (3)$ here I and I have dimensions of momentum and length respectively becomes (DPXxP) (DxxL) & t. DP'x ON 2 th here 12 has dimensions of th. This is uncertainty product in dimensionless form.

Programming

```
import numpy as np
2 import matplotlib.pyplot as plt
3 import scipy.integrate as integrate
4 import pandas as pd
{\tt 5} from scipy import optimize, stats
6 from IVP import RK_fourth_vec
7 def func_(x,x_vec,e):
      ans_vec = np.zeros((2))
      ans_vec[0] = x_vec[1]
9
      ans_vec[1] = (-e)*x_vec[0]
10
11
      return ans_vec
def analytical(x,n):
          if (i\%2) == 0:
              return 2*(np.cos(n*np.pi*x))**2
14
15
16
               return 2*(np.sin(n*np.pi*x))**2
17 def analytical_1(x,n):
return np.sin(n*np.pi*x)
E = np.linspace(0,400,100)
x = np.linspace(-1/2,1/2,100)
21 initcond = [0,1]
23 t = []
24 for i in range(len(E)):
      e = E[i]
      y1 = RK_fourth_vec(x, initcond, func_,e).T[0]
      y=y1/np.sqrt(integrate.simps(np.power(y1,2),x))
27
28
      t.append(y[-1])
29 # plt.scatter(E,t)
30 # plt.xlabel("e")
31 # plt.ylabel("$u_{R}$")
32 # plt.title("u(\u03BE=1/2)")
33 # plt.grid(True)
34 # plt.show()
35
36 def f(e,x):
      y1 = RK_fourth_vec(x, initcond, func_,e).T[0]
      y2 = RK_fourth_vec(x, initcond, func_,e).T[1]
38
      y=y1/np.sqrt(integrate.simps(np.power(y1,2),x))
40
      y_=y2/np.sqrt(integrate.simps(np.power(y2,2),x))
      t.append(y[-1])
41
      return t[-1], y,x,y_
42
43
44 en_neg = [];en_pos=[];i_neg=[];i_pos=[]
45 def eigenvalues(t):
      for i in range(1,len(t)):
46
47
          if t[i-1]*t[i]<0:</pre>
               en_neg.append(t[i-1])
48
               i_neg.append(E[i-1])
50
               en_pos.append(t[i])
51
               i_pos.append(E[i])
52
      return en_neg,en_pos,i_pos,i_neg
phi_1,phi_2,s_1,s_0 = eigenvalues(t)
55 data = {
      "u_1":phi_1,
      "E1":s_0,
57
      "u_2":phi_2,
58
      "E_2":s_1
59
60 }
#print(pd.DataFrame(data))
def secant(s_1,s_0,iterations,x):
      sec_2=[]
63
      sec_2.append(s_0); sec_2.append(s_1)
64
      for i in range(1,iterations):
```

```
sec_2.append(sec_2[i]-(((sec_2[i]-sec_2[i-1])*(f(sec_2[i],x)[0]))/((f(sec_2[i]-sec_2[i-1])))
66
       [i],x)[0])-(f(sec_2[i-1],x)[0]))))
           if abs(f(sec_2[-1],x)[0])<0.1e-12:</pre>
67
                return sec_2[-1], f(sec_2[-1],x)[0],f(sec_2[-1],x)[1],f(sec_2[-1],x)
68
       [2], f(sec_2[-1],x)[2]
69
70 E_n=[];u=[];v=[]
for i in range(0,len(s_0)):
       E_n=secant(s_1[i],s_0[i],501,x)[0]
73
74
       u_{-} = secant(s_{1}[i], s_{0}[i], 501, x)[1]
75
       ufull_ = secant(s_1[i], s_0[i], 501, x)[2]
       ufull_prime = secant(s_1[i], s_0[i], 501, x)[4]
76
77
       probability_density = secant(s_1[i],s_0[i],200,x)[3]
       x_{-} = secant(s_{1}[i], s_{0}[i], 501, x)[3]
78
79
       # plt.scatter(x_,ufull_,label=f'n={i+1}')
80
       # # plt.plot(x_,analytical_1(x_,i+1),label=f'n={i+1}')
       # plt.xlabel("\u03BE")
81
82
       # plt.ylabel("u(\u03BE)")
       # plt.title("Normalised wave function for infinite square well")
83
84
       # plt.grid()
       # plt.legend()
85
       # plt.show()
86
87
       # plt.scatter(x_,ufull_*ufull_,label=f'n={i+1}')
88
       # plt.plot(x_,analytical(x_,i+1),label=f'n={i+1}(Analytical)')
       # plt.xlabel("\u03BE")
90
91
       # plt.ylabel("$(u(\u03BE))^2$")
92
       # plt.title("Probability Densities")
       # plt.grid()
93
       # plt.legend()
94
       # plt.show()
95
96
97
       E_n.append(E_n_)
       u.append(u_)
98
       v.append(secant(s_1[i],s_0[i],200,x)[2])
99
101 print(E_n); print(u)
102
103
   data = {
       "N":[1,2,3,4,5,6],
104
       "Final Energy Eigen Value": E_n,
105
       "Corresponding u": u
106
107 }
print(pd.DataFrame(data))
slope, intercept, r, p, se = stats.linregress(np.array(E_n)/(np.pi)**2, E_n)
print("slope", slope)
# plt.scatter(np.array(E_n)/(np.pi)**2,E_n,label="Approximated")
# plt.plot(abs(np.array(E_n)/(np.pi)**2),(np.array(E_n)/(np.pi)**2)*(np.pi)**2,
       label="Analytical")
114 # plt.xlabel("$n^2$")
# plt.ylabel("$E_{n}$")
# plt.grid()
# plt.legend()
118 # plt.show()
120 def en_ev(E_n,h_cut,m_e,L):
       En_anal = []; prob_En_ev = []
121
       for i in range(0,len(E_n)):
122
           prob_En_ev_ = ((h_cut**2)*np.array(E_n)[i])/(2*m_e*(L**2)*(1.609e-19))
           prob_En_ev.append(prob_En_ev_)
124
125
           E = (((i+1)**2)*((np.pi)**2)*(h_cut**2))/(2*m_e*(L**2)*(1.609e-19))
           {\tt En\_anal.append(E)}
126
       return prob_En_ev, En_anal
m_e = 9.1e-31; h_cut = 1.0545e-34; m_p=1.6e-27
print("Well of width = 5 Angstrom")
```

```
130 data = {
       "Approximated Eigen Values": en_ev(E_n, h_cut,m_e,5e-10)[0],
131
       "Analytical Eigen Values": en_ev(E_n, h_cut,m_e,5e-10)[1],
132
133 }
print(pd.DataFrame(data))
135 print("
       ")
136 print("Well of width = 10 Angstrom")
137 data = {
       "Approximated Eigen Values": en_ev(E_n, h_cut, m_e, 10e-10)[0],
138
       "Analytical Eigen Values": en_ev(E_n, h_cut,m_e,10e-10)[1],
139
140 }
print(pd.DataFrame(data))
142
143 print("
      ")
144 print("Well of width = 5 Fermimeter for proton")
145 data = {
      "Approximated Eigen Values": en_ev(E_n, h_cut,m_p,5e-15)[0],
       "Analytical Eigen Values": en_ev(E_n, h_cut,m_p,5e-15)[1],
147
148 }
print(pd.DataFrame(data))
150
151 print("
      ")
152 '''Uncertainty Principle'''
153 exp_x_2=np.power(ufull_,2)*(np.power(x_,2))
i1=integrate.simps(exp_x_2,x_)
exp=np.power(ufull_,2)*(x_)
i2=integrate.simps(exp,x_)
157 variance = i1-i2**2
st_dev = np.sqrt(variance)
print("Uncertainty in x is ", np.sqrt(variance))
exp_x_p1 = np.power(ufull_prime,2)*x_
ip_1=integrate.simps(exp_x_p1,x_)
exp_x_p2=np.power(ufull_prime,2)*np.power(x_,2)
ip_2=integrate.simps(exp_x_p2,x_)
variance1=ip_2-ip_1**2
print("uncertainty in momentum p is", np.sqrt(variance1))
print("sigma_x*sigma_p = ",np.sqrt(variance)*np.sqrt(variance1))
167 print("h_cut/2*pi=",h_cut/(2))
168 print("sigma_x*sigma_p >= h_cut/2*pi, Hence Uncertainty Principle Verified ")
```

Result and Discussion

Here, We figure out the values of energy (e) and corresponding index ξ where u(ξ)) approaches zero.

PS C:\Users\adn19> & C:\Users\adn19\anaconda3\python.exe "d:\Sem 5\Quantum Mechanics\Lab\Assignments\Assignment 3\/1140_Preetp al_qmLab-A3.py"

	-	1.6		
	u_1	E1	u_2	E_2
0	0.397263	8.080808	-0.494418	12.121212
1	-0.347030	36.363636	0.104070	40.404040
2	0.296276	84.848485	-0.004676	88.888889
3	-0.019051	157.575758	0.207527	161.616162
4	0.012515	246.464646	-0.168943	250.505051
5	-0.142226	351.515152	0.009081	355.555556

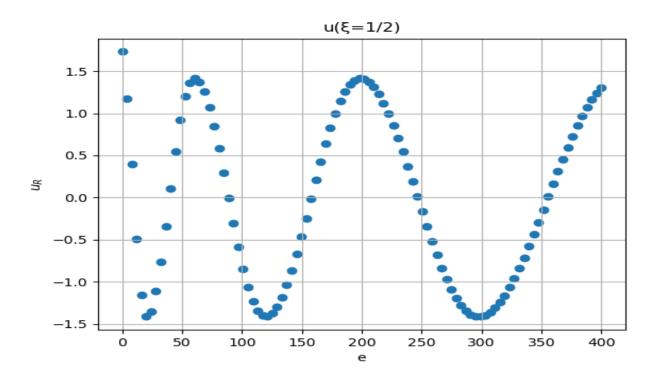
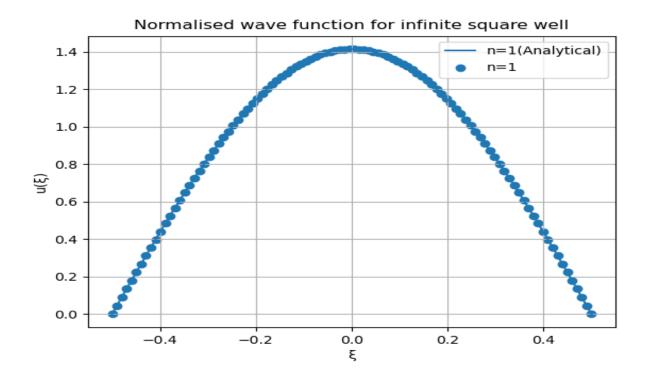
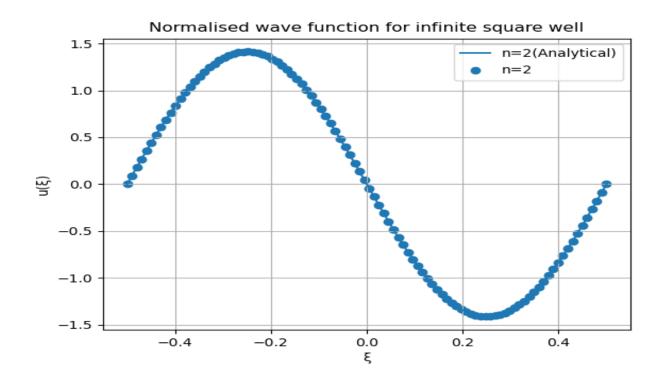


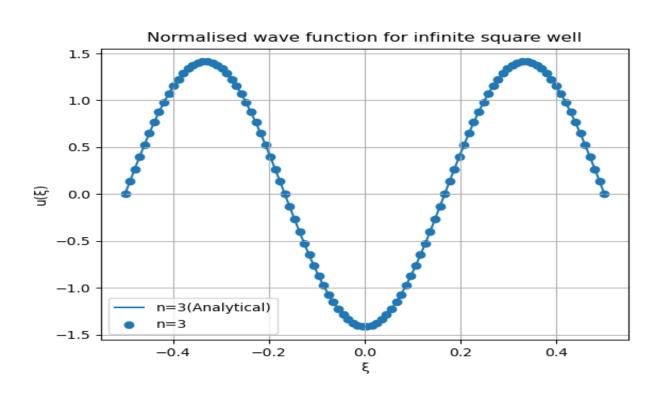
Figure 1: Plot between u_R and e to check where u_R approaches zero.

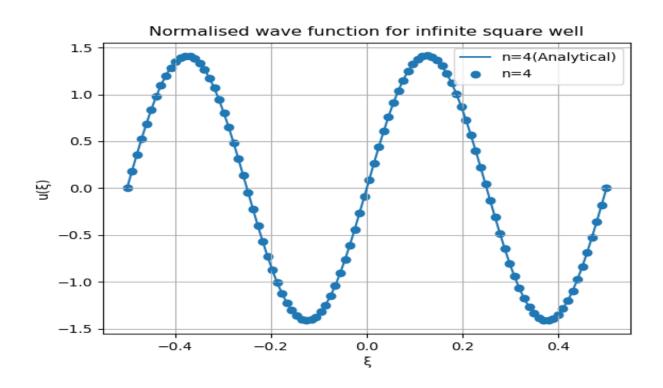
Normalised wavefunction for Infinite potential Well

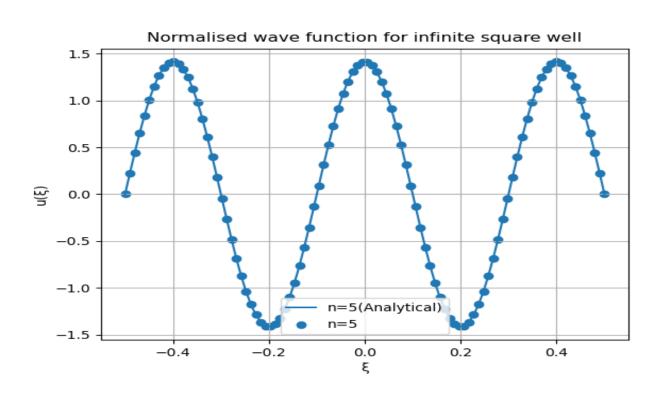
First, we predicted another values that closely approaches zero using shooting method to find energy eigen values. with this method, we find first 6 energy eigen values(Values of e where $u(\xi)$ corresponds to zero. Then using these eigen values, we plotted $u(\xi)$ vs ξ for different energy levels.

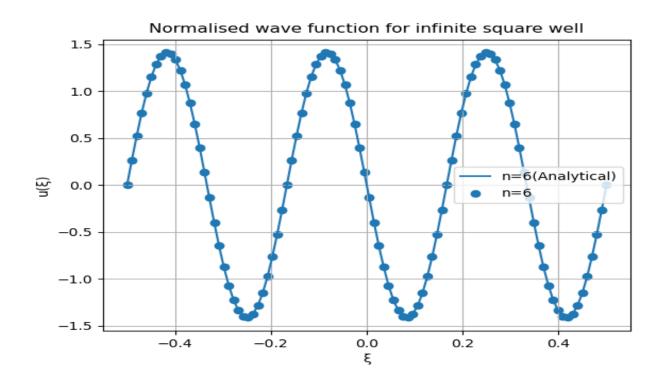




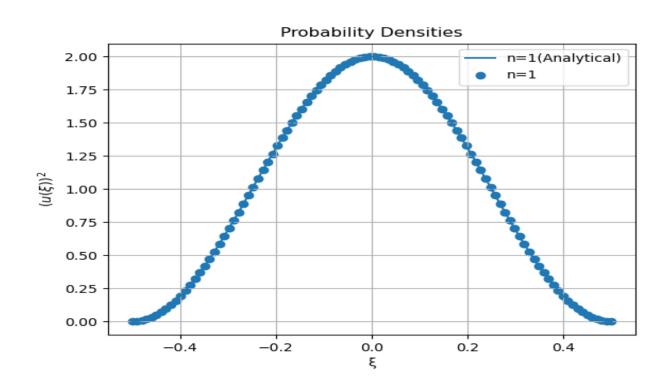


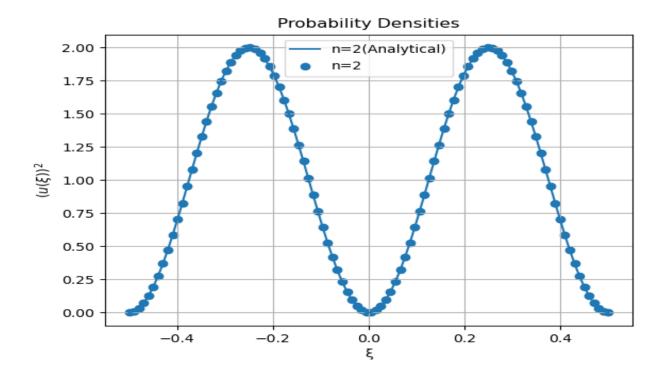


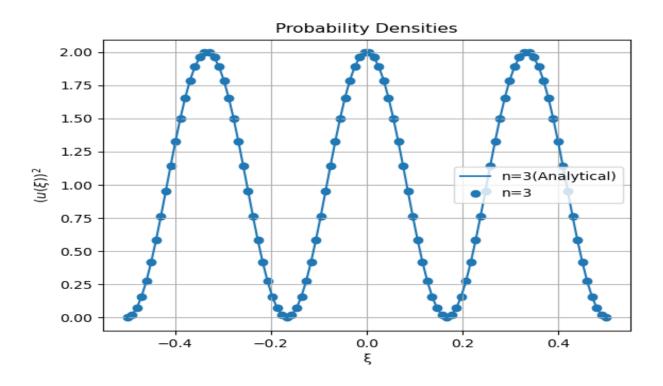


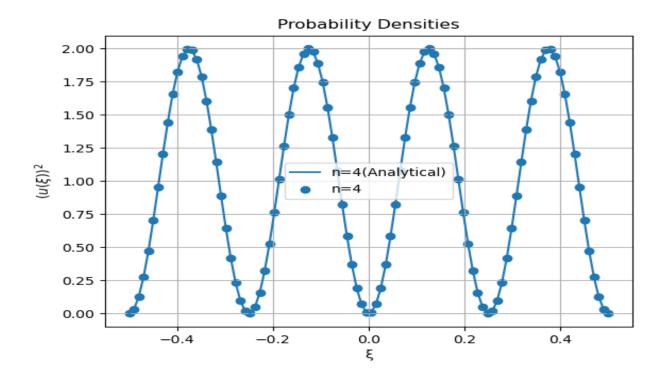


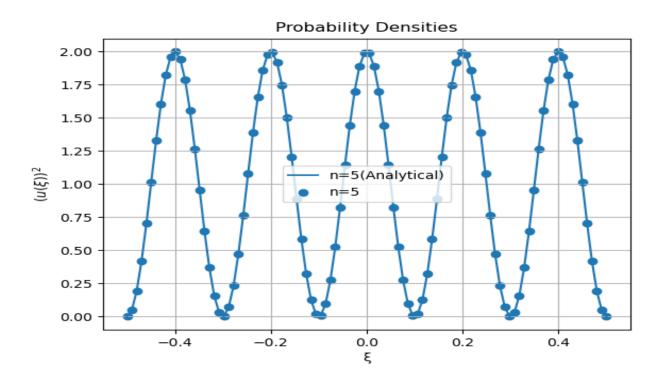
Normalised Probability Density for infinite square well

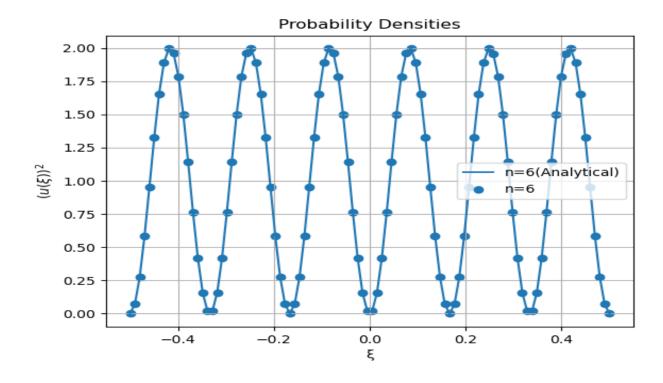












E_n vs n^2 Graph

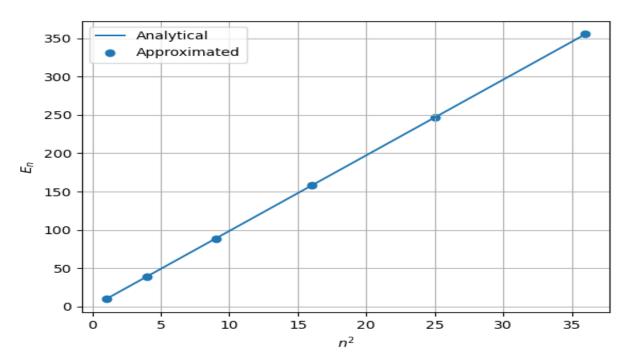


Figure 2: Here, Analytical solution and Numerical solutions matched. The Graph of E_n vs n^2 is linear in nature because $E_n = -n^2 \pi^2$.

```
N Final Energy Eigen Value Corresponding u
                          9.869605
                                       6.165728e-17
1
2
                        39.478428
                                       -3.015026e-14
   3
                        88.826561
                                        6.011509e-16
3
   4
                       157.914350
                                        -7.398713e-16
4
   5
                       246.742693
                                        -2.312080e-16
5
   6
                       355.313441
                                        1.387245e-16
slope 9.86960440108936
Well of width = 5 Angstrom
Approximated Eigen Values Analytical Eigen Values
0 1.499082 1.499082
                       5.996331
                                                     5.996329
2
                      13.491759
                                                   13.491741
                      23.985420
                                                   23.985317
4
                      37.477450
                                                   37.477057
5
                      53.968129
                                                   53,966962
Well of width = 10 Angstrom
   Approximated Eigen Values Analytical Eigen Values
0.374771 0.374771
                       1.499083
                                                     1.499082
2
                       3.372940
                                                     3.372935
                       5.996355
                                                     5.996329
                       9.369362
                                                     9.369264
5
                      13.492032
                                                   13.491741
Well of width = 5 Fermimeter for proton
   Approximated Eigen Values Analytical Eigen Values
0
                   8.526031e+06
                                                8.526031e+06
3.410412e+07
1
                   3.410413e+07
2
                   7.673438e+07
                                                7.673427e+07
3
                  1.364171e+08
                                                1.364165e+08
                   2.131530e+08
                                                2.131508e+08
                   3.069437e+08
                                                3.069371e+08
Uncertainty in x is 0.28626042521917944 uncertainty in momentum p is 0.11180453413430508
sigma_x*sigma_p = 0.03200521348271843
h_cut/2*pi= 5.2725e-35
sigma_x*sigma_p >= h_cut/2*pi, Hence Uncertainty Principle Verified
```