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2020PHY1216

LAB ASSIGNMENT - 08

Answer no. (a) :-

soln :- The Schrodinger Equation for 1-d in time - Indepedent form :-

$$\left[-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} + V(x)\,\psi(x) = E\,\psi(x) \quad -(1) \right]$$

where, $-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x) = H$

then Equation (1) becomes :-

$$H\psi = E\psi$$

In dimensionless form :-

$$Hu = -\frac{d^2u}{dx^2} + Vu = eu \quad -(2)$$

using taylor's expansion we can write :-

$$U(x+h) = u(x) + h\,u'(x) + \frac{h^2}{2!}u''(x) + \frac{h^3}{3!}u'''(x) + \cdots$$

$$+ \; u(x-h) = u(x) - h\,u'(x) + \frac{h^2}{2!}u''(x) - \frac{h^3}{3!}u'''(x) + \cdots$$

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In iterative form :-

$$u(x+h) = u(x_{i+1}) \quad \& \quad u(x) = u_i$$

4 by using central difference method :-

$$\left[\frac{d^2u}{dx^2} = \frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} \right]$$

Now putting this $\frac{d^2u}{dx^2}$ in equ^n ② !-

$$-\left(\frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} \right) + vu_i = eu_i$$

for $i = 1$

$$\Rightarrow -\left(\frac{u_2 - 2u_1 + u_0}{h^2} \right) + vu_1 = eu_1$$

but, $u_0 = 0$

$$\therefore \Rightarrow -\left(\frac{u_2 - 2u_1}{h^2} \right) + vu_1 = eu_1$$

for $i = 2$

$$\Rightarrow -\left(\frac{u_3 - 2u_2 + u_1}{h^2} \right) + vu_2 = eu_2$$

similarly !-

$$\Rightarrow -\left(\frac{u_4 - 2u_3 + u_2}{h^2} \right) + vu_3 = eu_3$$

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& for $i = 4$

$$= -\left(\frac{u_5 - 2u_4 + u_3}{h^2}\right) + v\, u_4 = e u_4$$

Now, writting all these equation's in matrix form :-

$$\Rightarrow -\frac{1}{h^2}\begin{bmatrix} -2u_1 & u_2 & 0 & 0 & 0 \\ u_1 & -2u_2 & u_3 & 0 & 0 \\ 0 & u_2 & -2u_3 & u_4 & 0 \\ 0 & 0 & u_3 & -2u_4 & u_5 \end{bmatrix}$$

$\&[u_5 = 0]$

$$+ \begin{bmatrix} v_1 & 0 & 0 & 0 \\ 0 & v_2 & 0 & 0 \\ 0 & 0 & v_3 & 0 \\ 0 & 0 & 0 & v_4 \end{bmatrix}\begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{bmatrix} = e\begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{bmatrix}$$

$\therefore$

$$\Rightarrow -\frac{1}{h^2}\begin{bmatrix} -2 & 1 & 0 & 0 \\ 1 & -2 & 1 & 0 \\ 0 & 1 & -2 & 1 \\ 0 & 0 & 1 & -2 \end{bmatrix}\begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{bmatrix}$$

$$+ \begin{bmatrix} v_1 & 0 & 0 & 0 \\ 0 & v_2 & 0 & 0 \\ 0 & 0 & v_3 & 0 \\ 0 & 0 & 0 & v_4 \end{bmatrix}\begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{bmatrix} = e\begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{bmatrix}$$

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(b)

Since, x is ranging from $-a/2$ to $a/2$

$\therefore$ $x = a$. let, $a = 1$

& it is given that internal grid point is 3 -

$\therefore$ $n = 3$

& $N = 3+1 = 4$

$\therefore$ $h = \frac{1}{N} = \frac{1}{4} = 0.25$

Since, the potential is given by :-

$$V(x) = \begin{cases} 0 & , -1/2 < x < 1/2 . \\ \infty & , \text{otherwise} . \end{cases}$$

from previous question :-

$$= \frac{-1}{(0.25)^2} \begin{bmatrix} -2 & 1 & 0 \\ 1 & -2 & 1 \\ 0 & \cancel{1} & -2 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix} + \begin{bmatrix} 0 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix}$$

$$= e \begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix}.$$

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$$\Rightarrow \begin{bmatrix} 32 & -16 & 0 \\ -16 & 32 & -16 \\ 0 & -16 & 32 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix} = e \begin{bmatrix} u_1 \\ u_2 \\ u_2 \end{bmatrix}$$

for eigen value's :-

$$\begin{vmatrix} 32-\lambda & -16 & 0 \\ -16 & 32-\lambda & -16 \\ 0 & -16 & 32-\lambda \end{vmatrix} = 0$$

$$(32-\lambda)\left[(32-\lambda)^2 - 256\right] + 16\left[-16(32-\lambda)\right] = 0$$

$$(32-\lambda)\left[(32-\lambda)^2 - 256 - 256\right] = 0$$

$$(32-\lambda)\left[\lambda^2 + 1024 - 64\lambda - 512\right] = 0$$

$$(32-\lambda)\left[\lambda^2 - 64\lambda + 512\right] = 0$$

$$(32-\lambda) = 0 \quad \& \quad \lambda^2 - 64\lambda + 512 = 0$$

$$\therefore \lambda_1 = 32 \quad \& \quad \lambda_2 = \frac{64 + 45.25}{2} \quad \& \quad \lambda_3 = \frac{64 - 45.25}{2}$$

$$\therefore \left[\lambda_1 = 32 \quad \& \quad \lambda_2 = 54.625 \quad \& \quad \lambda_3 = 9.37\right]$$

$\therefore$ The eigen value's are

$$\left[\lambda_1 = 9.37 \quad , \lambda_2 = 32 \quad \& \lambda_3 = 54.625\right]$$

Eigen vector for $\lambda = 9.37$

$$\begin{bmatrix} 22.63 & -16 & 0 \\ -16 & 22.63 & -16 \\ 0 & -16 & 22.63 \end{bmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

$$22.63\, x_1 - 16 x_2 = 0$$
$$-16 x_1 + 22.63 x_2 - 16 x_3 = 0$$
$$-16 x_2 + 22.63 x_3 = 0$$

on solving :-

$x_1 = x_3$
& $x_2 = 1.4159 x_3$

$$\therefore X_1 = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 1 \\ 1.4159 \\ 1 \end{pmatrix}$$

similarly :-
for $\lambda = 32$

$$X_2 = \begin{pmatrix} -1 \\ 0 \\ 1 \end{pmatrix}$$

& for $\lambda = 54.62$

$$X_3 = \begin{pmatrix} 1 \\ -\sqrt{2} \\ 1 \end{pmatrix}$$

$\therefore$ These X_1, X_2 & X_3 are eigen vectors.

1 Discussion

1. These are the waveform that we are getting across the corresponding states by solving the matrix formed.

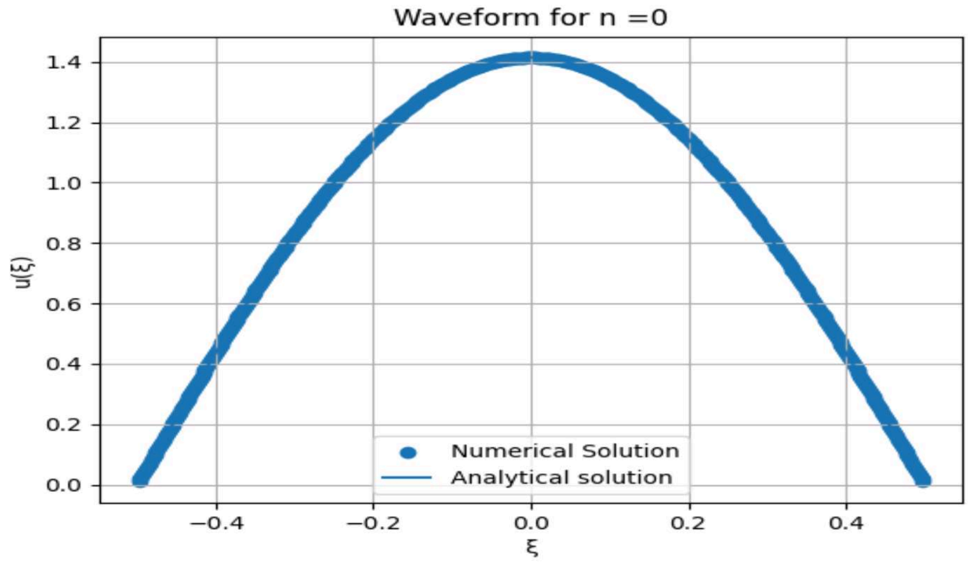

Figure 1:

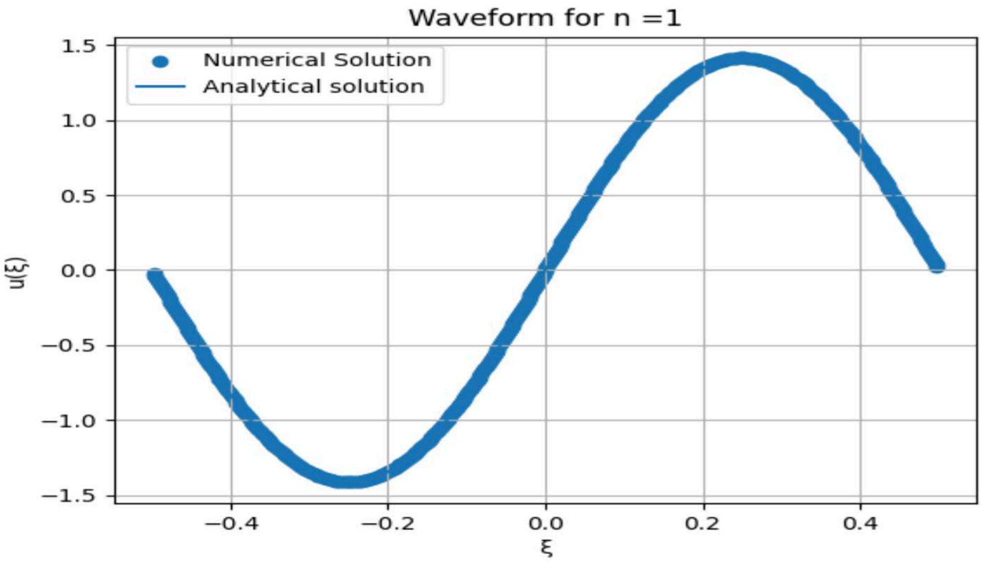

Figure 2:

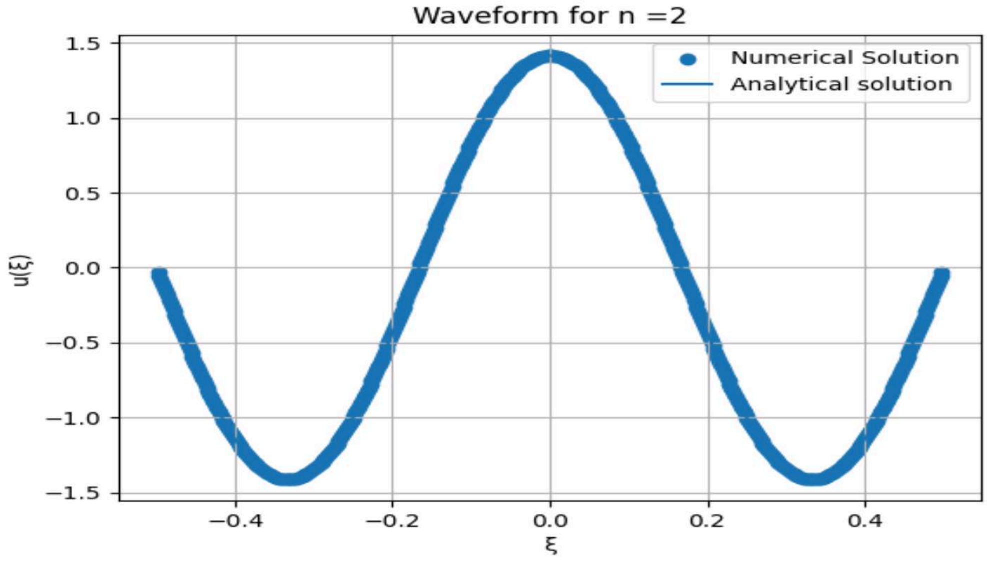

Figure 3:

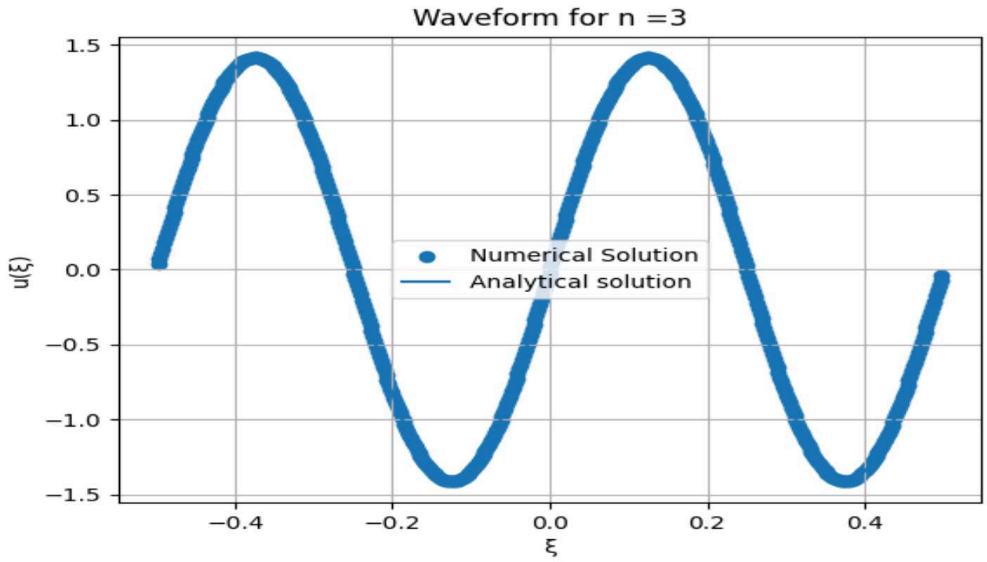

Figure 4:

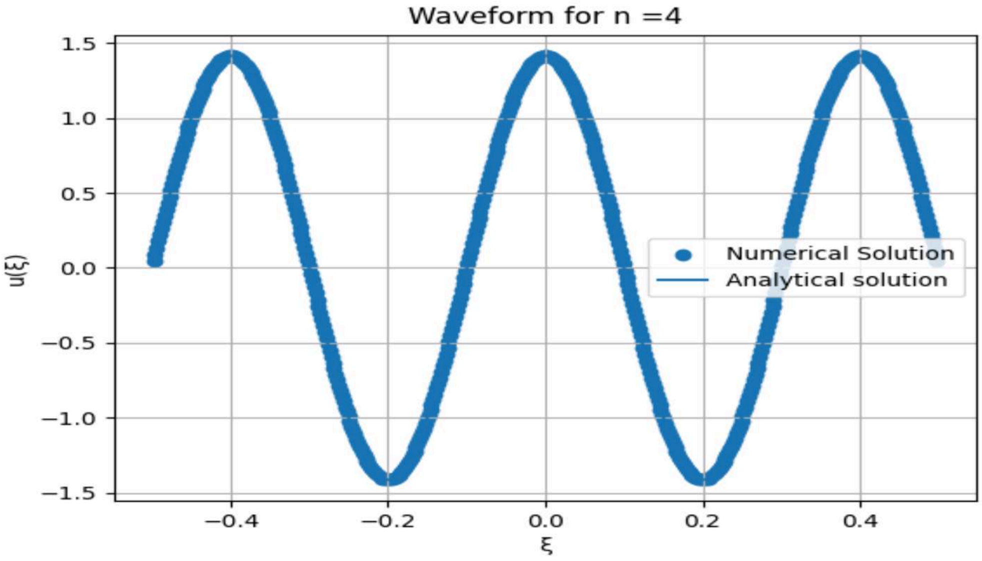

Figure 5:

2. In this part we are plotting the Probability Density for each state along with ξ

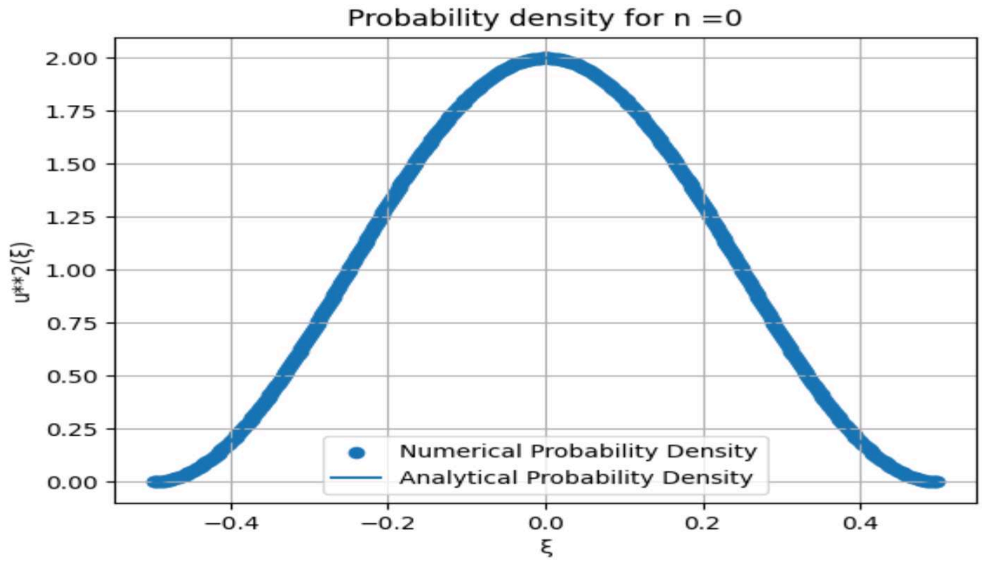

Figure 6:

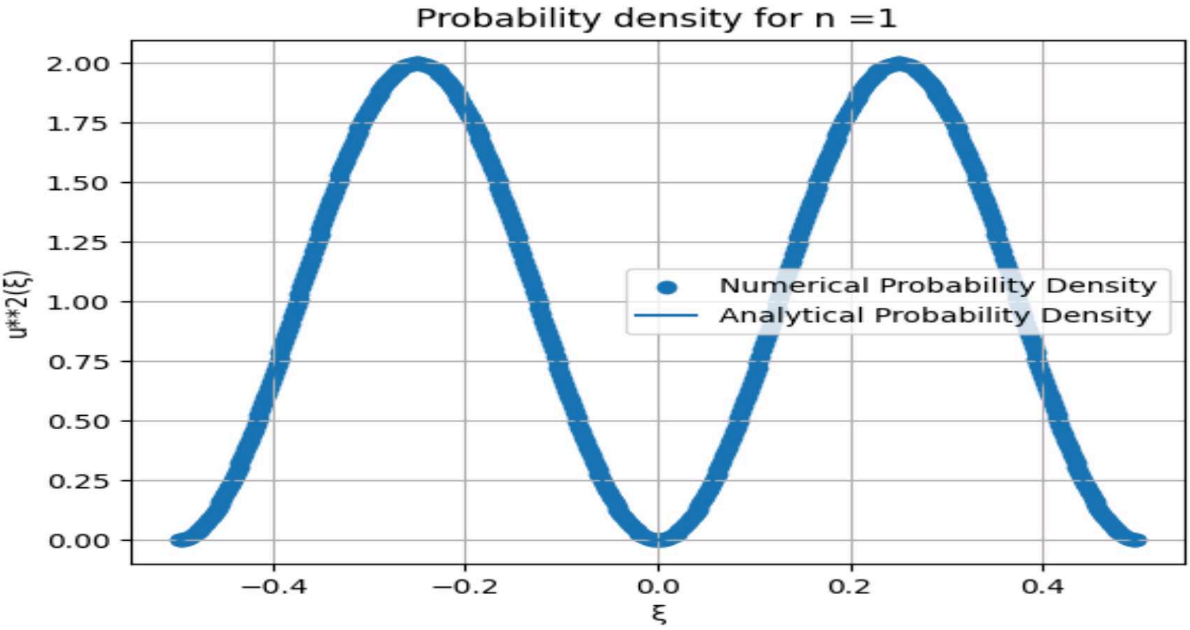

Figure 7:

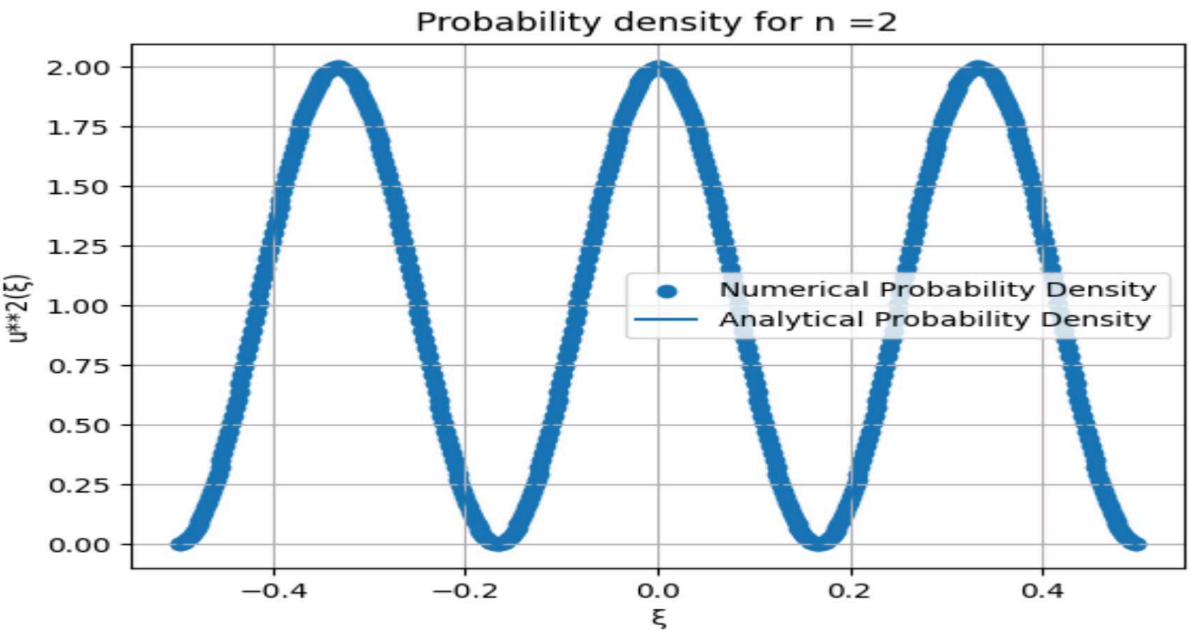

Figure 8:

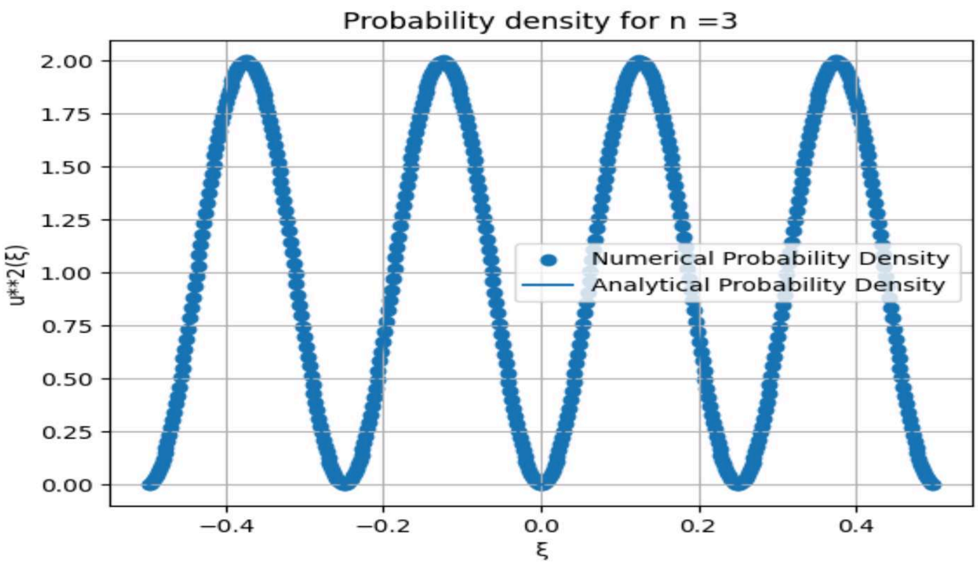

Figure 9:

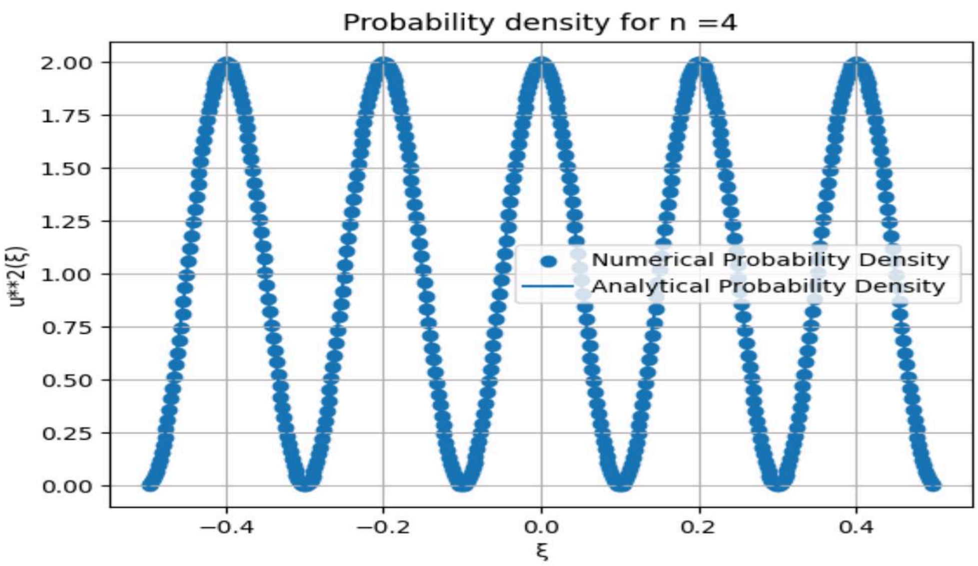

Figure 10:

3. These are the eigen values for the first ten states.

	Eigen Values
0	9.869572
1	39.477900
2	88.823820
3	157.905391
4	246.719898
5	355.263848
6	483.532972
7	631.522227
8	799.225795
9	986.637080

Figure 11:

B.Sc.(Hons.) Physics
32221501
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S.G.T.B. Khalsa College
Quantum Mechanics (2022-23)
Lab Assignment # 5
Finite Difference Method

Due Date and Time :
11.09.2022, 11:59PM
Max. Marks : 20

The objective of this assignment is to

- numerically solve the Schrödinger Equation for "particle in a box" problem with Finite Difference method and determine the energy eigenvalues and corresponding normalised wavefunctions for bound states.

1. (8 marks) **Theory**

   (a) Explain the finite difference method for solving the Time Independent Schrödinger Equation in 1-d.

   (b) An electron is confined in 1-d box from $x = -a/2$ to $a/2$. Show the numerical steps for finding its first two energy eigen values and the corresponding stationary state wavefunctions using the finite difference method with three internal grid points from $x = -a/2$ to $a/2$. Perform the calculations correct to four significant digits and compare with the analytical values.

2. (10 marks) **Programming**

   (a) Write a Python code to solve the Schrödinger Equation for the above problem by finite difference method and determine the first ten energy eigenvalues and normalised eigenfunctions .

   (b) Extend the code to plot the first four wavefunctions (as points) along with the corresponding analytical wavefunction (as continuous curves).

   (c) Plot the probability densities (as scatter plots) along with the analytical ones (as continuous curves) for all the four states in one plot.

3. (2 marks) **Discussion**
   Discuss your results and compare with those of the Shooting method (Assignment A3).