2020PHY1216

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LAB ASSIGNMENT -10

Answer (a) :-

Since, TISE is of the form :-

$$\nabla^2 \psi + \frac{2m}{\hbar^2}(E-V)\psi = 0$$

Now, we have to determine the Laplace operator in spherical coordinate :-

$$\because \quad x = r\sin\theta \cos\phi$$
$$y = r\sin\theta \cdot \sin\phi$$
$$z = r\cos\theta$$

$$\because \quad r^2 = x^2+y^2+z^2$$

$$\& \quad \tan\phi = y/x$$

Thus Schrodinger equ^n in Polar coordinate is :-

$$\left[\frac{1}{r^2}\frac{d}{dr}\left(r^2 \frac{\partial \psi}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{d}{d\theta}\left(\sin\theta \frac{\partial \psi}{\partial \theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2 \psi}{\partial \phi^2} + \frac{2m}{\hbar^2}(E-V)\psi = 0 \right]$$

This is schrodinger equ^n in spherical coordinate.

Since, S.E in polar form is

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right)+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right)+\frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial\phi^2}$$

$$+\frac{2m}{\hbar^2}(E-V)=0$$

Multiply by $r^2\sin\theta$:-

$$\sin^2\theta\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right)+\sin\theta\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right)+\frac{\partial^2\psi}{\partial\phi^2}$$

$$+\frac{2mr^2\sin^2\theta}{\hbar^2}(E-V)\psi=0 \quad \text{— (1)}$$

$\because$ ψ is $\psi(r,\theta,\phi)=R(r)\cdot P(\theta)\cdot\Theta(\phi)$. —(2)

Putting (2) in (1) :-

$$\frac{1}{R(r)}\sin^2\theta\frac{\partial}{\partial r}\left(r^2\frac{\partial R(r)}{\partial r}\right)+\frac{\sin\theta}{P(\theta)}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial P(\theta)}{\partial\theta}\right)$$

$$+\frac{1}{\Theta(\phi)}\frac{\partial^2\Theta_\phi}{\partial\phi^2}+\frac{2mr^2\sin^2\theta}{\hbar^2}(E-V)=0$$

$$\therefore \frac{\sin^2\theta}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \frac{\sin\theta}{P}\frac{d}{d\theta}\left(\sin\theta\frac{dP}{d\theta}\right) + \frac{2mr^2\sin^2\theta}{\hbar^2}(\varepsilon - V)$$

$$= -\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2}$$

$\because$ L.H.S depends on r & θ & R.H.S to ϕ but they are equal to same constant :-

$$\therefore \frac{\sin^2\theta}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \frac{\sin\theta}{P}\frac{d}{d\theta}\left(\sin\theta\frac{dP}{d\theta}\right) + \frac{2mr^2\sin^2\theta}{\hbar^2}(\varepsilon - V) = m^2$$

— (3)

dividing this by $\sin^2\theta$:-

$$\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \frac{2mr^2}{\hbar^2}(\varepsilon - V) = \frac{m^2}{\sin^2\theta} - \frac{1}{P\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{dP}{d\theta}\right)$$

— (4)

Now, again equating to a constant :-

$$\left[\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \frac{2mr^2}{\hbar^2}(\varepsilon - V) = l(l+1)\right]$$

— (5)

This is radial part.

(b)

Boundary conditions for numerical solution using RK4 :-

$$U(0) = 0$$
$$U'(0) = \text{arbitrary}.$$

It can be any value when the function is normalized.

Boundary conditions for numerical sol^n using Numerov :-

$$U(0) = 0$$
$$U(0+h) = h$$

'h' is the step size which is a small number.

1 Discussion

1. These are the Eigen Values for first five eigen states with $l = 0, 1, 2$ ..

	Enery for l = 0	Energy for l = 1	Energy for l = 2
0	-0.992816	0.000000	0.000000
1	-0.249941	-0.249989	0.000000
2	-0.111063	-0.111111	-0.111111
3	-0.062439	-0.062500	-0.062500
4	-0.039927	-0.040001	-0.040000

Figure 1:

2. This is the plot for the Radial Waveform for first four states .

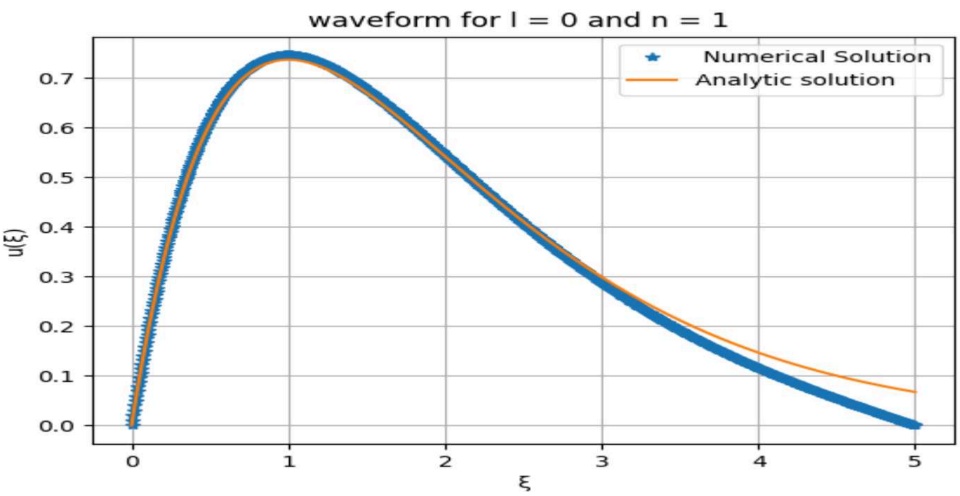

Figure 2:

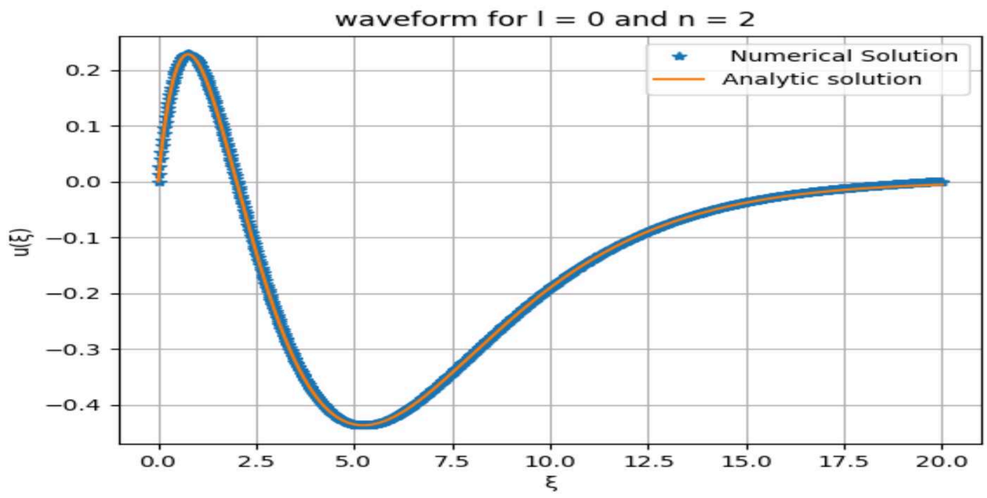

Figure 3:

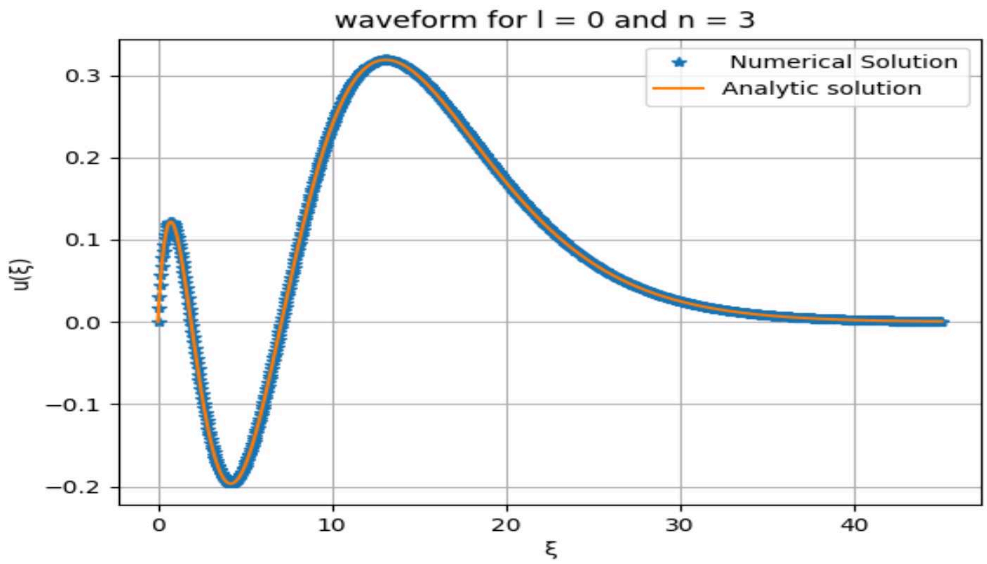

Figure 4:

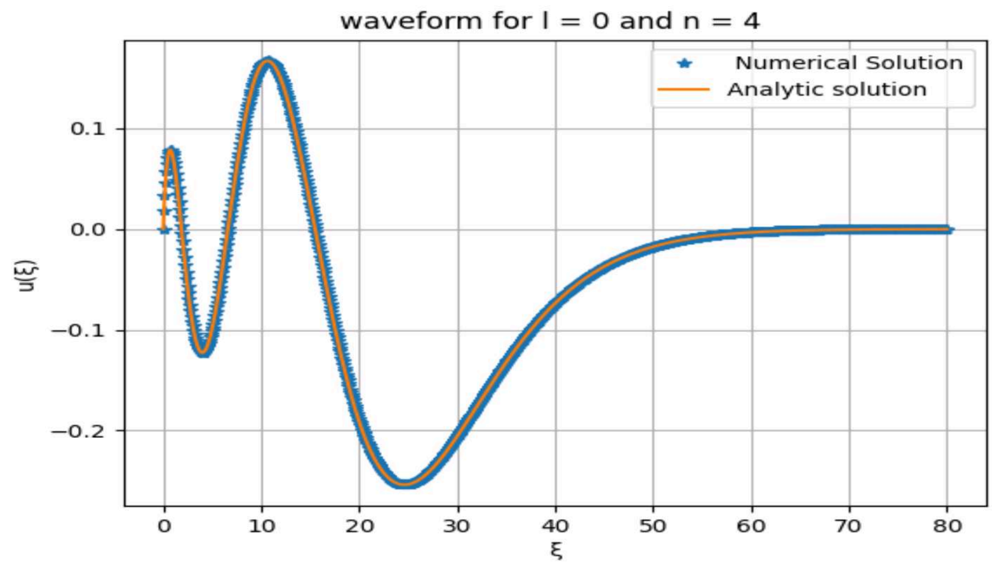

Figure 5:

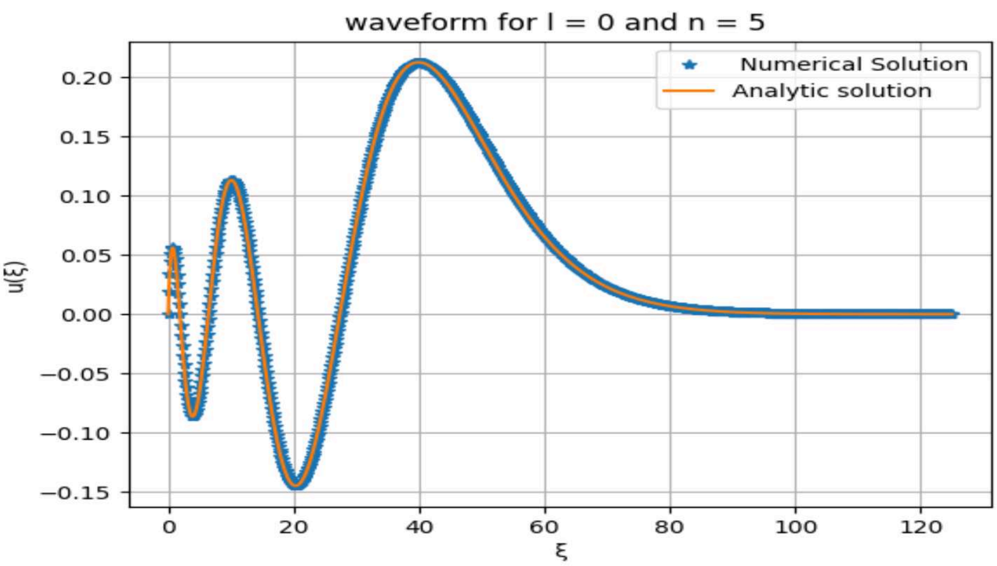

Figure 6:

3. The plots for Probability Density is here .

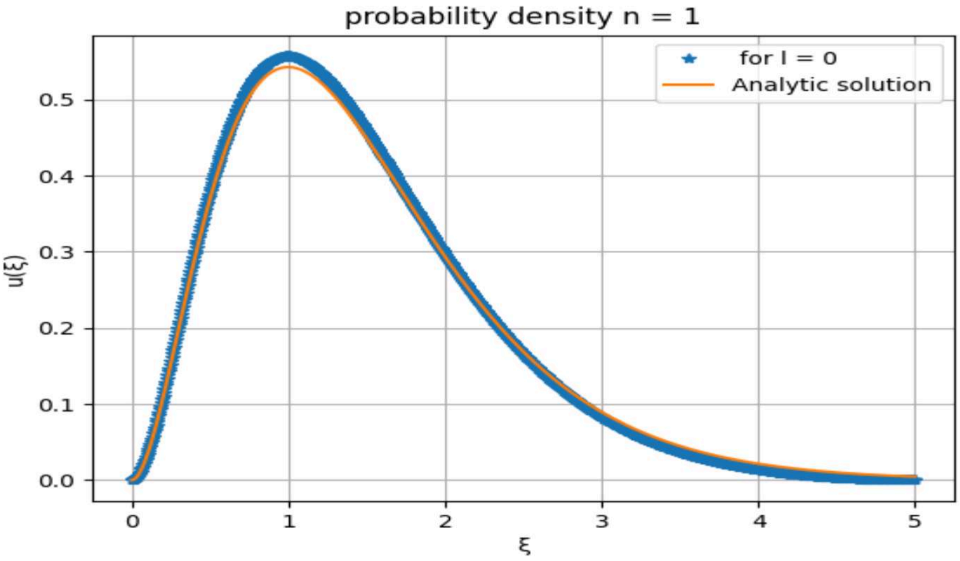

Figure 7:

B.Sc.(Hons.) Physics	**S.G.T.B. Khalsa College**	Due Date and Time :
32221501	**Quantum Mechanics (2022-23)**	22.09.2022, 11:59PM
Teacher: Mamta	**Lab Assignment # 10**	Max. Marks : 20
	H- atom using Shooting Method	

The objective of this assignment is to

- numerically solve the radial part of Schrödinger Equation for "electron in H-atom" with Shooting method and determine the energy eigenvalues and corresponding normalised radial wavefunctions.

1. (3 marks) **Theory**

   (a) Write down the Schrödinger Equation for an electron in H-atom potential in spherical polar coordinates and the equation satisfied by radial part of the wave

   (b) Discuss the boundary conditions for numerical solution using RK4 with shooting and Numerov with shooting methods.

2. (12 marks) **Programming**

   (a) Write a Python code to

      i. Determine the first ten energy eigenvalues and normalised radial wavefunctions for $\ell = 0$ using shooting method with Numerov algorithm in range $[r_{\text{min}} : r_{\text{max}}]$ with $r_{\text{min}} = 10^{-14}$ with $r_{\text{max}} = 10$.

      ii. plot the first four radial wavefunctions (as points) along with the corresponding analytical wavefunctions (as continuous curves).

   (b) Extend the code to determine the first ten energy eigenvalues and normalised eigenfunctions for $\ell = 1, 2$

   (c) Extend the code to plot all radial probability densities (as scatter plots) along with the corresponding analytical wavefunction (as continuous curves) for all ℓ corresponding to a given n. i.e. the following graphs

      i. radial probability density for $n = 1$, $\ell = 0$

      ii. radial probability density for $n = 2$, $\ell = 0$, 1

      iii. radial probability density for $n = 3$, $\ell = 0, 1$, 2

   (d) Study the implication of changing r_{min} and r_{max}.

   (e) Extend your program to determine the probability that an electron in 2s state of H-atom lies within a sphere of radius $r = pa_0$ around the nucleus. Take $p = 0.5$, 1, 1.5, 2, 3 4, $\ldots$, 10, 20, $\ldots$ 50 and show that the probability approaches 1 as p increases. Plot this probability as a function of p.

3. (5 marks) **Discussion**

   Discuss your results and compare with those of the Finite Difference Method.