Page No. 2020-011/216 Date: / # ASSIGNMENT -10 \$ LAB Answer (a):-Line, TISE of the form: -0 = y(v-3) 2m Rave to determine the Operator Now, sphenical Coondinate K= dsino cuso y = rsino sino 2 2 86030 12+42 + 22 tan 0 = yIx Palar coordinate Schredinger Thu (20h20 2m

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$ \frac{1}{R(6)} \frac{1}{\sqrt{3}} \frac{1}{\sqrt{3}} \left( \frac{8^{2} \sqrt{3} R(6)}{\sqrt{3}} \right) + \frac{\sin \theta}{\rho(6)} \frac{1}{\sqrt{3}} \left( \frac{\sin \theta}{\sqrt{3}} \frac{1}{\sqrt{6}} \right) \\ + \frac{1}{\sqrt{3}} \frac{1}{\sqrt{3}} \frac{1}{\sqrt{3}} \frac{1}{\sqrt{3}} + \frac{2m\chi^{2} \sin^{2} \theta}{\sqrt{3}} \left( \frac{\varepsilon}{2} - v \right) > 0 $ $ \frac{1}{\sqrt{3}} \frac{1}{$	1	Pulling (	2) in	(1) ! -					
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F	1 d (x2 dR) + 2mx2 (E-V) = l(1+1)
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parameter for recovery						

# 1 Discussion

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

	Enery for 1 = 0	Energy for 1 = 1	Energy for 1 = 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 .

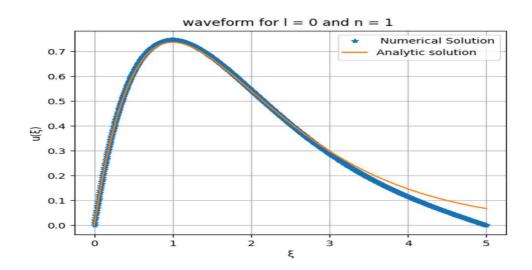


Figure 2:

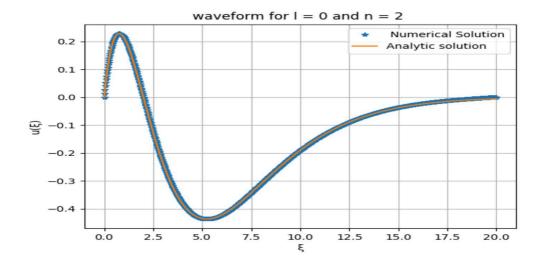


Figure 3:

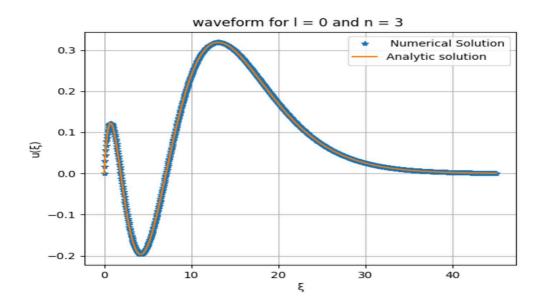


Figure 4:

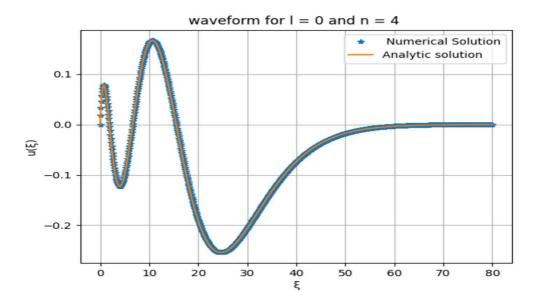


Figure 5:

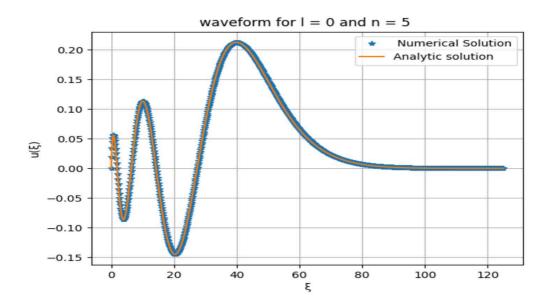


Figure 6:

3. The plots for Probability Density is here .

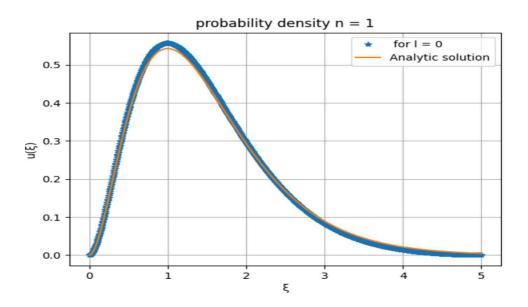


Figure 7:

B.Sc.(Hons.) Physics 32221501 Teacher: Mamta

## S.G.T.B. Khalsa College Quantum Mechanics (2022-23) Lab Assignment # 10 H- atom using Shooting Method

Due Date and Time: 22.09.2022, 11:59PM Max. Marks : 20

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  $[r_{\min}:r_{\max}]$  with  $r_{\min}=10^{-14}$  with  $r_{\max}=10$ .
  - 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  $\ell$  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, 34, ..., 10, 20, ... 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.