B.Sc.(Hons.) Physics	**S.G.T.B. Khalsa College**	
32221501	**Quantum Mechanics (2022-23)**	Due Date and Time :
Teacher: Mamta	**Lab Assignment # 10**	22.09.2022, 11:59PM
	H- atom using Shooting Method	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 ℓ corresponding to a given n. i.e. the following graphs

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

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

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

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

3. (5 marks) **Discussion**

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