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

**S.G.T.B. Khalsa College**
**Quantum Mechanics (2022-23)**
**Lab Assignment # 9**
**H- atom using Finite Difference Method**

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

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The objective of this assignment is to

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

1. (10 marks) **Theory**

   (a) Write down the Schrödinger Equation for an electron in H-atom potential in spherical polar coordinates.

   (b) Use separation of variable method to separate this into angular and radial part. (Use $\psi_{n\ell m}(r,\theta,\phi) = \mathcal{R}_{n\ell}(r)\mathcal{Y}_{\ell m}(\theta,\phi)$ and take the separation constant as $\ell(\ell+1)$. )

   (c) Convert the Radial part of the Schrödinger Equation dimensionless form. Take $\mathcal{R}_{n\ell}(r) = \mathcal{K}_{n\ell}(r)/r$ and write the equation satisfied by $\mathcal{K}_{n\ell}(r)$. For this rescale $r$ by Bohr radius and the energies by $|E_1|$, $E_1$ being the ground state Bohr energy.

   (d) Discuss $V_{\text{eff}}(x)$ and its implications.

   (e) Write down the analytical expressions for Bohr radius, Energy Eigenvalues and Energy eigenfunctions in this dimensionless form.

   (f) Discuss the boundary conditions for numerical solution using finite difference method.

2. (10 marks) **Programming**

   (a) Write a Python code to

      i. Plot $V(r)$ and $V_{\text{eff}}(r)$ as a function of $r$ for $\ell = 1, 2, 3$ on the same plot. Take range of $r$ to be $[r_{\min} : r_{\max}]$ with $r_{\min} = 10^{-14}$ and $r_{\max} = 50$, $r$ being the dimensionless variable.

      ii. Determine the first ten energy eigenvalues and normalised eigenfunctions for $\ell = 0$ using finite difference method with $r_{\max} = 10$

      iii. 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 $n = 0$, $\ell = 0$

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

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