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

S.G.T.B. Khalsa College
Quantum Mechanics (2022-23)
Lab Assignment # 2
Particle in a box - I

Due Date and Time :
01.08.2022, 11:59PM
Max. Marks : 20

The objective of this assignment is to

- review the shooting method for solving BVP.
- understand the hurdles in solving Schrödinger Equation .
- learn the importance of converting a physics problem to non-dimensional one for numerical work.
- discuss the solutions of Schrödinger Equation for a symmetric potential
- numerically solve the Schrödinger Equation for "particle in a box" problem and realise how the boundary conditions impose the discreteness in enrgy eigenvalues for bound states.

1. (8 marks) **Theory**
   (a) Write down the Schrödinger Equation for a quantum particle of mass m in a potential $V(x)$. Use separable of variables method to find the solution of the form $\Psi(x,t) = u(x)f(t)$ for the case when the potential is independent of time. Determine $f(t)$ and find the equation satisfied by the function $u(x)$?
   (b) If $V(x)$ is an even function of x, show that the solution of the TISE Schrödinger Equation can be taken to be either even or odd functions.
   (c) Solve the Schrödinger Equation for a particle in a 1-d box analytically in the range $\left[-\frac{L}{2} : \frac{L}{2}\right]$ i.e.
   $$V(x) = \begin{cases} 0 & \text{for} \quad |x| < \frac{L}{2} \\ \infty & \text{otherwise} \end{cases} \tag{1}$$
   (d) Convert the Schrodinger Equation for Infinite Potential well into Dimensionless form and write down the energy eigenvalues in dimensionless form (say e). How will you obtain the energy E in physical units from the numerical solution e in the dimensionless form.

2. (10 marks) **Programming**
   (a) Write a Python code to solve the Schrödinger Equation for electron (in dimensionless form) trapped in the potential given by (1) for a given value of e(energy in dimensionless form) using Runge Kutta method. The code should return the normalised wavefunction vector $u(\xi)$ where ξ is the dimensionless variable corresponding to x.
   (b) Take $e = 8$ and $u'(-1/2) = 1$ and solve Schrödinger Equation to obtain the solution. Normalise the wave function and plot it along with the analytical solution. Change $u'(-1/2)$ and repeat. What change do you see in the solution
   (c) Repeat for $e = 11$.
   (d) Now vary e in a loop in the range $[0.9\pi^2 : 1.1\pi^2]$ with small step size until $|u(1/2)| < 0.5 \times 10^{-10}$. Print this eigenvalue and plot the ground state normalised eigen function. Also print the energy eigenvalue in eV for electron trapped in a well of width 2 angstrom.
   (e) Extend your program to perform above computation for the first excited state.

3. (2 marks) **Discussion**
   Interpret and discuss your results.