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

# S.G.T.B. Khalsa College
## Quantum Mechanics (2022-23)
## Lab Assignment # 3
## Particle in a box - II

Due Date and Time : 07.08.2022, 11:59PM
Max. Marks : 20

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The objective of this assignment is to

- numerically solve the Schrödinger Equation for "particle in a box" problem using shooting method with Runge Kutta method to solve IVP and determine the energy eigenvalues and corresponding normalised wavefunctions for bound states.
- understand and verify numerically the position-moentum uncertainty principle.

1. (8 marks) **Theory**

   (a) A particle of mass $m$ is trapped in the infinite potential well given by

   $$V(x) = \begin{cases} 0 & \text{for} \quad |x| < \frac{L}{2} \\ \infty & \text{otherwise} \end{cases} \tag{1}$$

   Compute the probability of finding an electron in the range $[-\frac{L}{4} : \frac{L}{4}]$ when it is in the ground state of the above potential well.

   (b) Write down the position-momentum uncertainty relation.

   (c) i. Compute the expectation values $\left\langle \hat{X} \right\rangle$, $\left\langle \hat{P} \right\rangle$, $\left\langle \hat{X}^2 \right\rangle$, $\left\langle \hat{P}^2 \right\rangle$, $\Delta x$(or $\sigma_x$) and $\Delta p$(or $\sigma_p$) for the particle in the $n$th stationary state of the infinite potential well given by (1).

   ii. Which state comes closest to the uncertainty limit.

   iii. Write down the uncertainty product 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 well given by (1) using Shooting along with RK4 method based on the algorithm discussed in the Lab class held on August 8, 2022. The code should

   i. Plot the value of $u_R(u(\xi = 1/2))$ as a function of $e$ (energy in dimensionless form) for a large range.

   ii. Print the indices '$i$' of energy vector at which $u_R$ changes sign along with the corresponding values of energies (which will serve as the guess values for finding actual energy values).

   iii. Print the final energy eigen values and plot the corresponding normalised wavefunction vectors $u(\xi)$ (as scatter plot) along with the analytical wavefunctions (as continuous curves) at least for the first five bound states.

   (b) Extend your program to plot $e_n$ as a function of $n^2$, fit a linear curve, find slope and and compare its value with the actual value.

   (c) Plot the probability densities (as scatter plots) along with the analytical ones (as continuous curves) for all the five states in one plot.

   (d) Convert energies to eV for an electron trapped in a well of width 5 angstrom and print a table of energy eigenvalues in eV along with the analytical values. Format your print statement to print values only with six significant digits.

   (e) Repeat above step for an electron in a well of width 10 angstroms and a proton in a well of width 5 fermimeters.

   (f) Extend your program to compute the variances $\sigma_x$ and $\sigma_p$ and verify the uncertainty principle.

   (g) Extend your program to compute the probability of finding electron in the range $[-\frac{L}{4} : \frac{L}{4}]$ when it is in the ground state.

3. (2 marks) **Discussion**

   Interpret and discuss your results.