

The objective of this assignment is to

- numerically solve the Schrödinger Equation for "particle in a HO potential" problem with Numerov method and determine the energy eigenvalues and corresponding normalised wavefunctions for bound states.

1. (8 marks) **Theory**

A particle of mass m is subjected to the harmonic oscillator potential given by $V(x) = \frac{1}{2}m\omega^2x^2$.

- Convert the Schrödinger Equation for a quantum harmonic oscillator in dimensionless Form
- Obtain the classical turning points. Write down the analytical expressions for classical turning points and Energy Eigenvalues e_i in the dimensionless form.
- Write down the expressions of first five normalised Energy eigenfunctions u_i as a function of the dimensionless variable defined above.
- Interpret the non-zero value of the ground state energy.

2. (10 marks) **Programming**

- Write a Python code to solve the Schrödinger Equation for an electron subjected to the harmonic potential based on the Numerov algorithm as discussed in the class.
 - Take $e_n = n + \frac{1}{2} + \Delta e$ (in units of $\hbar\omega$) with $\Delta e = 10^{-2}, 10^{-4}, 10^{-6}, 10^{-8}$ and $n = 0$ and integrate from $x = 0$ to $x = x_{\max}$ using Numerov method to determine $u_0(x)$.
 - Use the even and odd property of the wave function to extend it in the range $[-x_{\max} : 0]$.
 - Plot the corresponding normalised wavefunction vectors $u_0(\xi)$ (as scatter plot) for all values of Δe along with the analytical wavefunction (as continuous curves).
 - Repeat for the first three excited states with $\Delta e = 10^{-6}$
- Plot the probability densities (as scatter plots) along with the analytical ones (as continuous curves) for all the four states in one plot with $\Delta e = 10^{-6}$.
- Convert energies to eV for an electron subjected to harmonic oscillator of frequency $\omega = 5.5 \times 10^{14}$ s and print a table of energy eigenvalues in eV along with the analytical values.
- Extend your program to compute the probability of finding electron in the classically forbidden region when it is in the ground state.

3. (2 marks) **Discussion**

Interpret and discuss your results.