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

S.G.T.B. Khalsa College
Quantum Mechanics (2022-23)
Lab Assignment # 13
Anharmonic Oscillator

Due Date and Time :
20.10.2022, 11:59PM
Max. Marks : 20

- The objective of this assignment is to estimate the eigenvalues and eigenvectors associated with the harmonic oscillator Hamiltonian perturbed with a cubic term.
- This assignment is based upon the problem 3 of the syllabus.

1. (6 marks) **Theory**
   A particle of mass μ constrained to move in 1-dimension is subjected to the potential

$$V(x) = \frac{1}{2}kx^2 + bx^3\,; \quad k = \mu\,\omega^2. \tag{1}$$

   (a) Convert the equation into a dimensionless form by defining $x = \xi x_0$, where $x_0 = \sqrt{\hbar/\mu\,\omega}$ and ξ is the dimensionless position variable. Also define dimensionless potential energy $v(\xi) = V(x_0\,\xi)/E_0$ and dimensionless energy eigenvalue $\epsilon = E/E_0$ where $E_0 = \frac{1}{2}\hbar\omega$ is the ground state energy of the harmonic oscillator.

   (b) Plot the potential energy $v(\xi)$ as a function of ξ for $\alpha = 0$ and $\alpha = 10^{-q}$ with $q = 0, 1, 2, 3, 4$, where $\alpha = \frac{bx_0}{k}$.

   (c) Discuss what do you expect for the bound state eigen values.

2. (12 marks) **Programming**

   (a) Write a Python code to solve the Schrödinger Equation for a particle of mass $\mu = 940\,\mathrm{MeV/c^2}$ subjected to the potential given in equation (1) using any method known to you giving reasons for your choice of method. The code should

      i. obtain the first ten energy eigenvalues ϵ_n for each value of α mentioned above.

      ii. print the eigen values obtained along with the values given by second order perturbation theory[1] in a tabulated form rounded off to the first six significant digits.

      iii. plot ϵ_n as a function of n and compare the behaviour with that for harmonic oscillator.

   (b) Extend your program to print the energy eigenvalues in MeV.

   (c) Further extend your program to

      i. obtain the first five normalised eigenfunctions (dimensionless form) and corresponding probability densities in the range $[-\xi_{\max} : \xi_{\max}]$ with an appropriate value of $\xi_{\max}$.

      ii. plot these normalised wavefunctions for $\alpha = 0, 0.01, 0.1$ (all wavefunctions for one α in one plot). Verify that $\alpha = 0$ gives the same result as for harmonic oscillator.

      iii. plot the probability densities similarly.

      iv. plot the probability densities in ground state for $\alpha = 0$ and $\alpha = 10^{-q}$ with $q = 0, 1, 2, 3, 4$.

      v. Repeat above for the first excited state.

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

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[1] The perturbation theory estimates the energy eigenvalues upto second order to be (the reference will be shared with you along with the assignment):

$$\epsilon_n = (2n+1) - \frac{1}{8}\alpha^2\left[15(2n+1)^2 + 7\right]$$