Quantum Mechanics and Spectroscopy
CHEM 3PA3
Assignment 7 **Name:** _____

1. A particle of mass m is confined in a one-dimensional box of length a. The state of the particle is given by the wavefunction $\Psi(x) = \frac{1}{3}\psi_1(x) + \frac{i}{3}\psi_3(x) - \left(\frac{7}{9}\right)^{1/2}\psi_5(x)$, where $\psi_n(x)$ is a normalized particle-in-a-box wavefunction corresponding to quantum number n.

   (a) Is the wavefunction $\Psi(x)$ normalized?

   (b) What will be the outcome when the energy of the particle is measured?

   (c) If more than one result is possible, what is the probability of obtaining each result?

   (d) What is the expectation value of the energy?

2. Consider a harmonic oscillator of mass m undergoing harmonic motion in two dimensions x and y. the potential energy is given by $V(x,y) = \frac{1}{2}k_x x^2 + \frac{1}{2}k_y y^2$.

   (a) Write the expression for the Hamiltonian operator of the system.

   (b) What are the general expressions for the energy levels and wavefunctions of the two-dimensional harmonic oscillator?

   (c) What is the zero-point energy?

   (d) Consider the energy level that has an energy 10 times greater than the zero-point energy. What is the degeneracy of this level if $k_x = k_y$?

3. Consider a particle in a one dimensional box from $x = 0$ to $x = a$ subject to a perturbation V_0,

$$V(x) = \begin{cases} V_0 & \frac{a}{4} < x < \frac{3a}{4} \\ 0 & 0 \le x \le \frac{a}{4} \quad \text{and} \quad \frac{3a}{4} \le x \le a \\ \infty & \text{otherwise} \end{cases}$$

   (a) Determine the energy of the first order perturbation.

   (b) What is the first order correction of the wavefunction?

   (c) Obtain the second order correction to the energy of the particle.

   (d) The exact ground-state energy is $5.750345\hbar^2/ma^2$, compare this with the energy perturbed at zero, first, and second order.