Quantum Mechanics and Spectroscopy
CHEM 3PA3
Assignment 5 **Name:** _____

1. Which of the following operators, $\hat{A}$, represent an observable of a particle in one dimension?

   (a) $\hat{A}\Psi(x) = \Psi^2(x) + \Psi^\star(x)$

   (b) $\hat{A}\Psi(x) = \cos(x)\Psi(x) + x\Psi(x)$

   (c) $\hat{A}\Psi(x) = \Psi'(x)$

2. Suppose the ground state wavefunction for a system is

$$\Psi(x) = \begin{cases} A(1-x^2) & -1 \leq x \leq +1 \\ 0 & \text{otherwise} \end{cases}$$

   (a) What is the normalization constant for this wavefunction?

   (b) What is the Hamiltonian for which this wavefunction is an eigenfunction? Assume that the zero of the potential energy is chosen so that $V(x=0) = 0$.

   (c) What is the zero-point energy of this Hamiltonian?

   (d) What is the kinetic energy of this system in the ground state?

   (e) What is the potential energy of this wavefunction?

   (f) How does the energy of this system change if a uniform electron field is imposed. That is, consider the perturbation $\Delta V = F \cdot x$. Write formulas for the second-order change in the energy and in the wavefunction.

3. Consider the following potential for a particle in a one-dimensional box:

$$V(x) = \begin{cases} \frac{V_0}{a}x & 0 \leq x \leq a \\ \infty & \text{otherwise} \end{cases}$$

   Calculate the total energy of the particle at first order.

4. Consider the anharmonic oscillator given by,

$$V(x) = \frac{1}{2}kx^2 + \frac{1}{6}\gamma_3 x^3 + \frac{1}{24}\gamma_4 x^4.$$

   Calculate the first order perturbation energy to the ground state using the harmonic oscillator as the unperturbed system.