BCHM 485 Midterm Exam #1 March 12, 2024 Problem 1. (30 points) Consider a particle of mass *m* in a 1-D box defined by the following potential energy: V(x) = 0 for  $0 \le x \le a$ , and  $V(x) = \infty$  for x < 0 and x > a. The particle is in a state described by the following (unnormalized) wave function:  $\Psi(x) = \sqrt{\frac{2}{a}} \left[ 4\sin\left(\frac{3\pi}{a}x\right) - 3\sin\left(\frac{5\pi}{a}x\right) \right]$ . Answer the

following questions.

A. List all values of the energy of the particle that one can obtain in a single measurement in this state and the corresponding probabilities to measure these values.

**B.** Calculate the average value of the energy of the particle that will be measured as a result of multiple measurements in this state.

C. List all values of the momentum of the particle that one can obtain in a single measurement in this state and the average value of the momentum that will be measured as a result of multiple measurements.

**Problem 2.** (15 points) Is it possible to know with arbitrary precision both the angular coordinate  $\phi$  and the angular momentum  $l_z$  of a particle moving on a ring? Support your answer by evaluating the corresponding commutator. Based on your results, formulate a mathematical equation representing the uncertainty principle for these two observables.

**Problem 3.** (25 points) A quantum mechanical harmonic oscillator with mass  $\mu$  and force (spring) constant *k* is in a state characterized by the quantum number n = 2. A. Write the expression for the probability density to find the oscillator at a given value of coordinate *x*.

**B**. Determine the nodes, i.e. the values of coordinate x at which there is zero probability to find the oscillator.

**C.** Where are you more likely to find the quantum mechanical oscillator: at the very bottom of the potential well (i.e. at x = 0) or at the turning points of the classical oscillator (where its total energy equals its potential energy, i.e.,  $E_n = \frac{kx^2}{2}$ )? Support your answer by calculating the corresponding probability

densities.

**Problem 4. (30 points)** Consider a chlorine molecule (Cl<sub>2</sub>) in gas phase. Assume that there is no coupling between the translational, vibrational, and rotational states, i.e. these motions are independent from each other. You studied this molecule and obtained the following results: the quantum of energy absorbed upon transition from the ground state to the first excited rotational state is  $9.6864 \times 10^{-24}$  J; the quantum of energy required for a transition from the ground state to the first vibrational state is  $1.112 \times 10^{-20}$  J. Answer the following questions. The atomic mass of Cl is 35 a.m.u.

**A.** From these data, determine the equilibrium bond length in the molecule. Explain your assumptions.

**B.** Determine the force (spring) constant for the Cl-Cl bond. Explain your assumptions.

**C.** Assume the chlorine molecule is placed in a 3-D box/cube of size 10 Å (1 Å= $10^{-10}$  m). Calculate the energy of the ground state of translational motion of the molecule in that box.