Chem 21a: Assignment #4
Assigned: October 24, 2007
Due: October 31, 2007 @ 1pm

## <u>Rotational Motion, and the Hydrogen Atom</u>

**1.** *Molecular Quantum Mechanics*, page 96 problem 3.29

**2.** *Molecular Quantum Mechanics*, page 97 problem 3.31

**3. Uncertainty Principle for Particle on a Ring.**

**a.** Show explicitly in a basis of eigenfunctions of the z component of angular momentum ($L_z$) that the commatator relation:

$$\left[\hat{L}_z, \hat{\phi}\right] = -i\hbar$$

holds for motion of a particle of mass m on a circle of radius $R$ on the interval [0, 2π]. $\phi$ is the angular position operator for the particle.

**b.** Use the above relation to derive the result:

$$\frac{d}{dt}\langle n|\hat{\phi}|m\rangle = \frac{n\hbar}{mR^2} = \frac{L_z}{I}$$

for a particle on a ring, which is the Erhenfest relation corresponding to the classical result:

$$L = I\omega$$

where ω is the angular velocity and I the moment of inertia for the particle on a ring.

**4. Rigid Rotator and Particle on a Ring**.

A good model for the rotational behavior of diatomic molecules is the rigid rotor. In this model, the molecule is treated as two point masses $m_1$ and $m_2$ connected by a rigid, massless bond of fixed length R. The molecule is free to rotate in any direction about its center of mass.

*A. Derive the classical expression for the kinetic energy of a rigid rotator, as described above, which is undergoing uniform rotation about a fixed axis. You may assume that you are in an "inertial" reference frame in which the center of mass of the rigid rotator is stationary. Formulate your answer in terms of the moment of inertia, I, and angular momentum, L.*

*B. From your classical expression for the kinetic energy, write down the associated quantum mechanical Hamiltonian for the rigid rotator.*

*C. What are the eigenfunctions of this Hamiltonian, and what are the associated energy levels?*

A gyroscope can be treated as a particle on a ring and will have quantized rotational energy.

*D. For a "macroscopic" gyroscope having a moment of inertia of 2.5 g $cm^2$ rotating at an angular velocity of 100 rad/ s, calculate the rotational quantum number, m, and the minimum allowed change in rotational energy and angular velocity. Ignore precession and nutation, and give the positive value for m. (Hint: consider the similarity between the particle on a ring and the rigid rotor.)*

*E. The JPL microdevices lab has recently developed "micro" gyroscopes for use in altitude control on spacecraft. Assume a microgyro can be represented by a particle of mass $4 \times 10^{-18}$ kg with $r \approx 1$ μm rotating at an angular velocity of 200 rad/ s. Calculate the rotational quantum number, minimum rotational velocity change and minimum energy changes for the microgyro.*

**5. Electron in a Sphere (25 pts).**

An electron is trapped in a spherical box of radius a, defined by the potential V(r), which is infinite outside the sphere and zero within it:

$$\{V(r)=1, r>a; V(r)=0, r<a\}.$$

Determine the normalized radial solution and bound eigenvalues for the case $l$ = 0. You have seen the relevant radial equation in class and may find the substitution u(r)=rR(r) where R(r) is the is radial solution  convenient.

**Please write how much time you spent on this assignment at the top of your paper. This will help us keep the length of the assignments reasonable.**