Fall 2011 CHEM 760: Introductory Quantum Chemistry

Homework 4 Due Tuesday Oct 18, in class

Vectors

1. a) Determine $w = u \times v$ given that $u = -i + 2j + k$ and $v = 3i - j + 2k$.

   b) What is $v \times u$ equal to?

   c) Find the angle between the two vectors $u = -i + 2j + k$ and $v = 3i - j + 2k$.

2. Show that the set of vectors is orthonormal

   $\left(\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, 0, \frac{1}{\sqrt{3}}\right)$, $\left(\frac{1}{\sqrt{3}}, -\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, 0\right)$, $\left(0, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, -\frac{1}{\sqrt{3}}\right)$, and $\left(\frac{1}{\sqrt{3}}, 0, -\frac{1}{\sqrt{3}}, -\frac{1}{\sqrt{3}}\right)$

3. Show that

   $\frac{d}{dt}(u \cdot v) = \frac{du}{dt} \cdot v + u \cdot \frac{dv}{dt}$ and

   $\frac{d}{dt}(u \times v) = \frac{du}{dt} \times v + u \times \frac{dv}{dt}$

   (Hint, let $u = u_x(t)i + u_y(t)j + u_z(t)k$, and $v = v_x(t)i + v_y(t)j + v_z(t)k$)

4. a) Textbook (Levine's 6th ed. Quantum Chemistry) Prob. 5.18 (a)

   b) Textbook Prob. 5.19 (a)

Angular Momentum

5. Textbook Prob. 5.29
6. Textbook Prob. 5.34
7. Prove that $\hat{L}^2$ commutes with $\hat{L}_x, \hat{L}_y$ and $\hat{L}_z$.
8. In the far infrared spectrum of $H^{79}Br$, there is a series of lines separated by 16.72 cm^{-1}. Calculate the values of the moment of inertia and the internuclear separation in $H^{79}Br$.
9. The following lines were observed in the microwave absorption spectrum of $H^{127}I$ and $D^{127}I$ between 60 cm^{-1} and 90 cm^{-1}. Use the rigid-rotator approximation to determine the values of $\tilde{B}$, I and J for each molecule. Take the masses of H, D and ^{127}I to be 1.008, 2.013 and 126.904 amu, respectively.

	$\bar{\nu}_{obs}$ / cm^{-1}			
$H^{127}I$	64.275	77.130	89.985	
$D^{127}I$	65.070	71.577	78.094	84.591