Homework H16 Solution

1. Turn in
a) Prove that $Y_{1-1} - Y_{11}$ is also an eigenfunction of $\hat{H}_{rot}$. **Hint:** if each function in a sum has the same eigenvalue of energy, what is the energy of the sum?

b) Plot $Y_{1-1} - Y_{11}$ in the x-y plane ($\theta = \pi/2$, plot as function of $\varphi$). **Hint:** It is real.

**Solution:**
a. We know, $\hat{H}_{rot} Y_{l,m}(\theta, \varphi) = E_l Y_{l,m}(\theta, \varphi)$ where $E_l = \frac{\hbar^2}{2mr^2} l(l+1)$. Hence,

$$\hat{H}_{rot}(Y_{1-1} - Y_{11}) = \hat{H}_{rot} Y_{1,-1} - \hat{H}_{rot} Y_{1,1} = E_1 Y_{1,-1} - E_1 Y_{1,1} \text{ [where } E_1 = \frac{\hbar^2}{mr^2}]$$

Thus it’s an Eigenfunction of $\hat{H}_{rot}$ because $l=1$ for both functions, and the energy only depends on $l$, not $m$.

b. $Y_{l,m} = \mp \frac{1}{\sqrt{2\pi}} e^{\pm i \varphi} \sin \theta$

Considering $\theta = \frac{\pi}{2}$, $f=(Y_{1,-1} - Y_{1,1}) = \sqrt{\frac{3}{2\pi}} \cos \varphi$, which is real. The plot of $f$ vs. $\varphi \in [0,2\pi]$ should look like: …and the polar plot $r=f(\theta,\varphi)$ in the x-y plane:

2. Do problem 5.2 in the book.

Solution: The rotational energy is given by $E = \frac{\hbar^2}{2J} J(J+1)$, where $I = \mu r^2$. $I$ is called “the moment of inertia” of the molecule. Instead of “$L$” or “$l$”, physical chemists like to use the letter “$J$” for the rotational quantum number, so the magnitude of the rotational angular momentum is $|L|=\hbar\sqrt{J(J+1)}$. 
For HCl, \( \mu = \frac{1.008+34.97}{1.008+34.97} \times 10^{-3} \text{kg/mole} = 1.626 \times 10^{-27} \text{kg/molecule} \), \( r = 0.1275 \text{ nm} \), so

\[
l = \mu r^2 = 1.626 \times 10^{-27} \times (0.1275 \times 10^{-9})^2 = 2.64 \times 10^{-47} \text{kg m}^2
\]

For J=0 to J=1 transition,

\[
\Delta E = \frac{\hbar^2}{2l} (2 - 0) \quad (1)
\]

\[
= \frac{(6.626 \times 10^{-34})^2 \times 2}{2 \times 4 \times \pi^2 \times 2.64 \times 10^{-47}}
\]

\[
= 4.21 \times 10^{-22} J
\]

\[
\lambda = \frac{hc}{\Delta E} = \frac{6.626 \times 10^{-34} \times 3 \times 10^8}{4.21 \times 10^{-22}} = 4.72 \times 10^{-4} m
\]

Note that the answer in the book is off by a factor of 2. Their algebra error occurred because they forgot the factors of two cancel in the kinetic energy equation (1). Happens to the best!