Homework H16 Solution

1. **Turn in**

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

Solution:

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

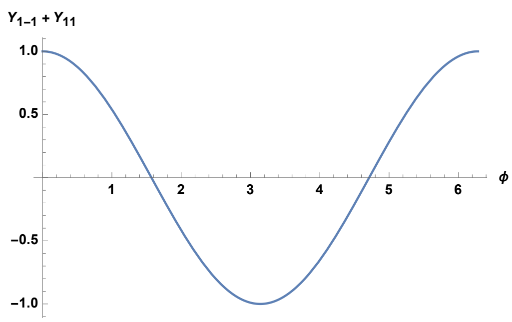
Hence,

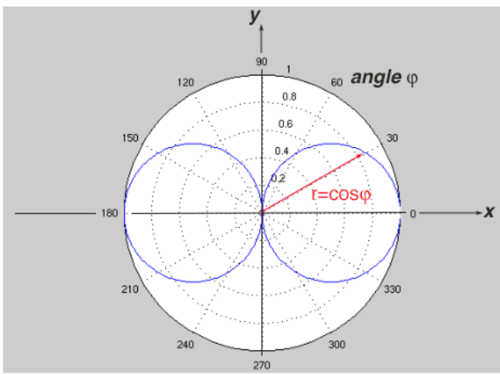
$$\hat{H}_{rot}(Y_{1\text{-}1} - Y_{11}) = \hat{H}_{rot} Y_{1,-1} - \hat{H}_{rot} Y_{1,1}$$
$$= E_1\, Y_{1,-1} - E_1\, Y_{1,1} \quad [\text{where } E_1 = \frac{\hbar^2}{mr^2}]$$
$$= E_1\,(Y_{1\text{-}1} - Y_{11}).$$

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

b. $Y_{1,\pm 1} = \mp\frac{1}{2}\sqrt{\frac{3}{2\pi}}\, e^{\pm i\varphi} sin\theta$

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(θ,φ) in the x-y plane:





2. Do problem 5.2 in the book.

Solution: The rotational energy is given by $E = \frac{\hbar^2}{2I}J(J+1)$, 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, $\mu = \frac{1.008*34.97}{1.008+34.97} * \frac{10^{-3}kg}{mole} = 1.626 * 10^{-27} kg/molecule$, r = 0.1275 nm, so

$$I = \mu r^2 = 1.626 * 10^{-27} * (0.1275 * 10^{-9})^2 = 2.64 * 10^{-47} kgm^2$$

For J=0 to J=1 transition,

$$\Delta E = \frac{\hbar^2}{2I}(2-0) \qquad (1)$$

$$= \frac{(6.626 * 10^{-34})^2 * 2}{2 * 4 * \pi^2 * 2.64 * 10^{-47}}$$

$$= 4.21 * 10^{-22} J$$

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

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!