CHEM 6472: Quantum Chem and Spectroscopy

Problem Set VII

Due Tues, Nov 26

1. Using

$$\hat{L}_x = \hat{Y}\hat{P}_z - \hat{Z}\hat{P}_y \tag{1}$$
$$\hat{L}_y = \hat{Z}\hat{P}_x - \hat{X}\hat{P}_z \tag{2}$$
$$\hat{L}_z = \hat{X}\hat{P}_y - \hat{Y}\hat{P}_x \tag{3}$$

and

$$[\hat{X}, \hat{P}_x] = i\hbar \tag{4}$$
$$[\hat{Y}, \hat{P}_y] = i\hbar \tag{5}$$
$$[\hat{Z}, \hat{P}_z] = i\hbar \tag{6}$$

show that the raising and lowering operators

$$\hat{L}_\pm = \hat{L}_x \pm i\hat{L}_y \tag{7}$$

satisfy

$$[\hat{L}_z, \hat{L}_\pm] = \pm\hbar\hat{L}_\pm \tag{8}$$

and

$$[\hat{L}^2, \hat{L}_\pm] = 0 \tag{9}$$

where $\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$.

2. Show that

$$Y_2^1(\theta, \phi) = -(15/8\pi)^{1/2} sin\theta\, cos\theta\, e^{i\phi} \tag{10}$$

is an eigenfunction of $\hat{L}_z$ with eigenvalue $\hbar$ and an eigenfunction of $\hat{L}^2$ with eigenvalue $6\hbar^2$. Then show that this function is normalized by integrating over the angular coordinates.

3. To a good approximation, the microwave spectrum of $H^{35}Cl$ consists of a series of equally spaced lines, separated by 6.26×10^{11} Hz. Using the *correct* reduced mass, calculate the bond length of $H^{35}Cl$.