Homework #5 Blake Evans

① Prove the following identity:

$$(1) \quad p \times L + L \times p = 2i\hbar p$$

$$(2) \quad i\hbar(p \times L - L \times p) = [L^2, p]$$

(1) we know that $\begin{cases} \vec{p} = p_x\hat{x} + p_y\hat{y} + p_z\hat{z} \\ \vec{L} = \vec{r} \times \vec{p} = L_x\hat{x} + L_y\hat{y} + L_z\hat{z} \end{cases}$

So, we can say

$$\vec{p} \times \vec{L} + \vec{L} \times \vec{p} = (p_x\hat{x} + p_y\hat{y} + p_z\hat{z}) \times (L_x\hat{x} + L_y\hat{y} + L_z\hat{z}) + (L_x\hat{x} + L_y\hat{y} + L_z\hat{z}) \times (p_x\hat{x} + p_y\hat{y} + p_z\hat{z})$$

$$= (p_xL_y\hat{z} - p_xL_z\hat{y} - p_yL_x\hat{z} + p_yL_z\hat{x} + p_zL_x\hat{y} + p_zL_y\hat{x})$$

$$+ (L_xp_y\hat{z} - L_xp_z\hat{y} - L_yp_x\hat{z} + L_yp_z\hat{x} + L_zp_x\hat{y} + L_zp_y\hat{x})$$

Now let's arrange this equation by $\hat{x}$, $\hat{y}$, and $\hat{z}$ to simplify our expression.

$$\vec{p}\times\vec{L}+\vec{L}\times\vec{p} = [p_yL_z + L_yp_z - p_zL_y - L_zp_y]\,\hat{x}$$

$$+ [p_xL_y - L_yp_x + p_xL_z - L_xp_z]\,\hat{y}$$

$$+ [p_xL_y + L_xp_y + p_yL_x - L_yp_x]\,\hat{z}$$

Now let's simplify

$$\hat{x}: \; [\underbrace{\boxed{p_yL_z - L_zp_y}}_{[p_y,\, L_z]} + \underbrace{\boxed{L_yp_z - p_zL_y}}_{[L_y,\, p_z]}]$$

$$\hat{y}: \; [\underbrace{\boxed{p_zL_x - L_xp_z}}_{[p_z,\, L_x]} + \underbrace{\boxed{L_zp_x - p_xL_z}}_{[L_z,\, p_x]}]$$

$$\hat{z}: \; [\underbrace{\boxed{p_xL_x - L_yp_x}}_{[p_x,\, L_y]} + \underbrace{\boxed{L_xp_y - p_yL_x}}_{[L_x,\, p_y]}]$$

Now let's calculate all the commutators

$$[P_y, L_z] = \boxed{-[L_z, P_y] = -\left(\hbar^2 \frac{\partial}{\partial x}\right)} = \hbar \frac{\partial}{\partial x}$$

$$[L_y, P_z] = \hbar^2 \left(\frac{\partial}{\partial x}\right)$$

$$[P_z, L_x] = \boxed{-[L_x, P_z] = -\left(\hbar^2 \frac{\partial}{\partial y}\right)} = \hbar^2 \frac{\partial}{\partial y}$$

$$[L_z, P_x] = \hbar^2 \frac{\partial}{\partial y}$$

$$[P_x, L_y] = \boxed{-[L_y, P_x] = -\left(\hbar^2 \frac{\partial}{\partial z}\right)} = \hbar^2 \frac{\partial}{\partial z}$$

$$[L_x, P_y] = \hbar^2 \frac{\partial}{\partial z}$$

Plug them all in

$$\left[\hbar^2 \frac{\partial}{\partial x}\right] + \left[\hbar^2 \frac{\partial}{\partial x}\right] + \left[\hbar^2 \frac{\partial}{\partial y}\right] + \left[\hbar^2 \frac{\partial}{\partial y}\right]$$
$$+ \left[\hbar^2 \frac{\partial}{\partial z}\right] + \left[\hbar^2 \frac{\partial}{\partial z}\right]$$

$$= \left(2\hbar^2 \frac{\partial}{\partial x}\right)\hat{x} + \left(2\hbar^2 \frac{\partial}{\partial y}\right)\hat{y} + \left(2\hbar^2 \frac{\partial}{\partial z}\right)\hat{z}$$

let $i^2 = -1$, we can re-write,

$$= -2i\hbar\left(i\hbar \frac{\partial}{\partial x}\hat{x} + i\hbar \frac{\partial}{\partial y}\hat{y} + i\hbar \frac{\partial}{\partial z}\hat{z}\right)$$

we know that $\vec{p} = i\hbar\left(\frac{\partial}{\partial x}\hat{x} + \frac{\partial}{\partial y}\hat{y} + \frac{\partial}{\partial z}\hat{z}\right)$
so we can say that

$$\boxed{\vec{p} \times \vec{L} + \vec{L} \times \vec{p} = -2i\hbar\,\vec{p}}$$

(2) we know that $\begin{cases} \vec{p} = p_x\hat{x} + p_y\hat{y} + p_z\hat{z} \\ \vec{L} = \vec{r} \times \vec{p} = L_x\hat{x} + L_y\hat{y} + L_z\hat{z} \end{cases}$

So, we can say

$$\vec{p} \times \vec{L} + \vec{L} \times \vec{p} = (p_x\hat{x} + p_y\hat{y} + p_z\hat{z}) \times (L_x\hat{x} + L_y\hat{y} + L_z\hat{z})$$
$$- (L_x\hat{x} + L_y\hat{y} + L_z\hat{z}) \times (p_x\hat{x} + p_y\hat{y} + p_z\hat{z})$$

$$= (p_xL_y\hat{z} - p_xL_z\hat{y} - p_yL_x\hat{z} + p_yL_z\hat{x} + p_zL_x\hat{y} + p_zL_y\hat{x})$$

$$-(L_xp_y\hat{z} - L_xp_z\hat{y} - L_yp_x\hat{z} + L_yp_z\hat{x} + L_zp_x\hat{y} + L_zp_y\hat{x})$$

$$\vec{p} \times \vec{L} - \vec{L} \times \vec{p} = [p_yL_z + L_zp_y - L_yp_z - p_zL_y]\,\hat{x}$$

$$+ [p_zL_x + L_xp_z - p_xL_z - L_zp_x]\,\hat{y}$$

$$+ [p_xL_y + L_yp_x - p_yL_x - L_xp_y]\,\hat{z}$$

Now let's expand the right side using the identity for [AB, CD].

$$[L^2, P] = \vec{L}^2 \vec{P} - \vec{P} L^2$$

$$= (L_x^2 + L_y^2 + L_z^2)(P_x \hat{x} + P_y \hat{y} + P_z \hat{z})$$

$$- (P_x \hat{x} + P_y \hat{y} + P_z \hat{z})(L_x^2 + L_y^2 + L_z^2)$$

$$\begin{aligned}
= \; & \cancel{L_x^2 P_x \hat{x}} && + L_x^2 P_y \hat{y} && + L_x^2 P_z \hat{z} \\
+ \; & L_y^2 P_x \hat{x} && + \cancel{L_y^2 P_y \hat{y}} && + L_y^2 P_z \hat{z} \\
+ \; & L_z^2 P_x \hat{x} && + L_z^2 P_y \hat{y} && + \cancel{L_z^2 P_z \hat{z}} \\
+ \; & \cancel{P_x L_x^2 \hat{x}} && + P_y L_x^2 \hat{y} && + P_z L_x^2 \hat{z} \\
+ \; & P_x L_y^2 \hat{x} && + \cancel{P_y L_y^2 \hat{y}} && + P_z L_y^2 \hat{z} \\
+ \; & P_x L_z^2 \hat{x} && + P_y L_z^2 \hat{y} && + \cancel{P_z L_z^2 \hat{z}}
\end{aligned}$$

All terms of same dependence cancel out. We are left with

$$\hat{x} : \left[\underbrace{\boxed{L_y^2 P_x - P_x L_y^2}}_{[L_y^2,\, P_x]} + \underbrace{\boxed{L_z^2 P_x - P_x L_z^2}}_{[L_z^2,\, P_x]}\right]$$

$$\hat{y} : \left[\underbrace{\boxed{L_x^2 P_y - P_y L_x^2}}_{[L_x^2,\, P_y]} + \underbrace{\boxed{L_z^2 P_y - P_y L_z^2}}_{[L_z^2,\, P_y]}\right]$$

$$\hat{z} : \left[\underbrace{\boxed{L_x^2 P_z - P_z L_x^2}}_{[L_x^2,\, P_z]} + \underbrace{\boxed{L_y^2 P_z - P_z L_y^2}}_{[L_y^2,\, P_z]}\right]$$

$$= \Big[\big(L_y[L_y, P_x] + [L_y, P_x]L_y\big)$$

$$+ \big(L_z[L_z, P_y] + [L_z, P_y]L_z\big)\Big]\hat{x}$$

$$+ \Big[\big(L_x[L_x, P_y] + [L_x, P_y]L_x\big)$$

$$+ \big(L_z[L_z, P_y] + [L_z, P_y]L_z\big)\Big]\hat{y}$$

$$+ \Big[\big(L_x[L_x, P_z] + [L_x, P_z]L_x\big)$$

$$+ \big(L_y[L_y, P_z] + [L_y, P_z]L_y\big)\Big]\hat{z}$$

we can simplify

$$x : \left[L_y\left(-\hbar^2 \frac{\partial}{\partial z}\right) + \left(-\hbar^2 \frac{\partial}{\partial z}\right) L_y\right]$$

$$+ \left[L_z\left(\hbar^2 \frac{\partial}{\partial y}\right) + \left(\hbar^2 \frac{\partial}{\partial y}\right) L_z\right]$$

$$= \left[-i\hbar\left(-L_y p_z - p_z L_y\right)\right] + \left[i\hbar\left(L_z p_y + p_y L_z\right)\right]$$

$$y : \left[L_x\left(\hbar^2 \frac{\partial}{\partial x}\right) + \left(\hbar^2 \frac{\partial}{\partial x}\right) L_x\right]$$

$$+ \left[L_z\left(-\hbar \frac{\partial}{\partial x}\right) + \left(-\hbar \frac{\partial}{\partial x}\right) L_z\right]$$

$$= \left[i\hbar\left(L_x p_z + p_z L_x\right)\right] + \left[i\hbar\left(-L_z p_x - p_x L_z\right)\right]$$

$$z : \left[L_x\left(-\hbar^2 \frac{\partial}{\partial y}\right) + \left(-\hbar^2 \frac{\partial}{\partial y}\right) L_x\right]$$

$$+ \left[L_y\left(\hbar^2 \frac{\partial}{\partial x}\right) + \left(\hbar^2 \frac{\partial}{\partial x}\right) L_y\right]$$

$$= \left[i\hbar\left(-L_x p_y - p_y L_x\right)\right] + \left[i\hbar\left(L_y p_x - p_x L_y\right)\right]$$

Finally, if we combine terms we can see

$$= i\hbar\left[p_y L_z + L_z p_y - L_y p_z - p_z L_y\right]\hat{x}$$

$$+ i\hbar\left[p_z L_x + L_x p_z - p_x L_z - L_z p_x\right]\hat{y}$$

$$+ i\hbar\left[p_x L_y + L_y p_x - p_y L_x - L_x p_y\right]\hat{z}$$

This is the same as what we had before.

$$\vec{p}\times\vec{L}-\vec{L}\times\vec{p} = \left[p_y L_z + L_z p_y - L_y p_z - p_z L_y\right]\hat{x}$$

$$+\left[p_z L_x + L_x p_z - p_x L_z - L_z p_x\right]\hat{y}$$

$$+\left[p_x L_y + L_y p_x - p_y L_x - L_x p_y\right]\hat{z}$$

② For a CO_2 molecule, calculate the first 3 rotational energy levels.

From class, we know that $E_n = B\,n(n+1)$

where $B = \dfrac{\hbar^2}{2I}$ and $I = \mu r^2$ (moment of inertia)

reduced mass

The reduced mass (μ) of CO_2 is given by

$$\mu = \frac{m_C m_{O_2}}{m_C + m_{O_2}} = \frac{(12.01\text{ amu})(31.99\text{ amu})}{(12.01\text{ amu}) + (31.99\text{ amu})}$$

$$\mu = 8.73\ \cancel{\text{amu}}\left(\frac{1.66\times10^{-27}\text{ kg}}{1\ \cancel{\text{amu}}}\right)$$

$$\mu = 1.45\times10^{-26}\text{ kg}$$

The bond length of CO_2 is $r = 116\times10^{-12}$ m

we can put this together to get

$$I = \mu r^2 = (1.45\times10^{-26}\text{ kg})(116\times10^{-12}\text{ m})^2$$

$$I = 1.95 \times 10^{-46}\ kg \cdot m^2$$

Then, we can plug this into our equation for B.

$$B = \frac{\hbar^2}{2I} = \frac{(1.054 \times 10^{-34}\ J \cdot s)^2}{2(1.95 \times 10^{-46}\ kg \cdot m^2)} \qquad J = \frac{kg \cdot m^2}{s^2}$$

$$B = 2.85 \times 10^{-23}\ J \left(\frac{\cancel{kg \cdot m^2}}{\cancel{s^2}}\right) s^2 \left(\frac{1}{\cancel{kg \cdot m^2}}\right)$$

$$B = 2.85 \times 10^{-23}\ J \quad \text{or} \quad 1.78 \times 10^{-4}\ eV$$

And finally, we can calculate the first 3 rotational energies.

$$E_{(1)} = (1.78 \times 10^{-4}\ ev)(1)((1)+1) = \boxed{3.54 \times 10^{-4}\ eV}$$

$$E_{(2)} = (1.78 \times 10^{-4}\ ev)(2)((2)+1) = \boxed{1.07 \times 10^{-3}\ eV}$$

$$E_{(3)} = (1.78 \times 10^{-4}\ ev)(3)((3)+1) = \boxed{2.14 \times 10^{-3}\ eV}$$

③ Consider a spin-$3/2$ system

(a) write down S^2 and S_z^2 in the S_z basis

a spin $3/2$ system has four possible states: $3/2, 1/2, -1/2, -3/2$.

The four eigenstates are

$|s m_s\rangle = |3/2, 3/2\rangle, |3/2, 1/2\rangle, |3/2, 1/2\rangle, |3/2, 3/2\rangle$

The eigenvalue equation for S^2 is,

$S^2|s m_s\rangle = s(s+1)\hbar^2|s m_s\rangle = 15/4\,\hbar^2|3/2, m_s\rangle$

The eigenvalue equations for S_z is

$S_z|s m_s\rangle = m_s\hbar|s m_s\rangle$

$$\boxed{S_z|s m_s\rangle = \begin{array}{l} 3/2\,\hbar\,|3/2, 3/2\rangle \\ 1/2\,\hbar\,|3/2, 1/2\rangle \\ -1/2\,\hbar\,|3/2, -1/2\rangle \\ -3/2\,\hbar\,|3/2, -3/2\rangle \end{array}}$$

(b) $S_\pm = S_x \pm i S_y$. show that

$$S_\pm |s m_s\rangle = \hbar\sqrt{s(s+1)-m_s(m_s\pm1)}\,|s, m_s\pm1\rangle$$

we know $S^2|s,m_s\rangle = s(s+1)\hbar^2$

$S_z|s,m_s\rangle = m_s\hbar$

Let's let $|\psi\rangle = S_+|s,m_s\rangle = \beta|s,(m_s+1)\rangle$
and perform $\langle\psi|\psi\rangle$.

$$\langle\psi|\psi\rangle = \langle s,m_s|(S_+)^\dagger S_+|s,m_s\rangle = \beta|s,(m_s+1)\rangle$$

we know that $(S_+)^\dagger = S_-$, so

$$\langle s,(m+1)|\beta|s,(m+1)\rangle = \langle s,m_s|S_-S_+|s,m_s\rangle$$

$$\beta\underbrace{\langle s,(m+1)|s,(m+1)\rangle}_{1} = \langle s,m_s|S_-S_+|s,m_s\rangle$$

Now let's expand S_-S_+.

$$S_-S_+ = (S_x - iS_y)(S_x + iS_y)$$

$$= S_x^2 + iS_xS_y - iS_yS_x - i^2S_y^2$$

$$= S_x^2 + S_y^2 + i[S_x, S_y]$$

$$= S_x^2 + S_y^2 + i(i\hbar S_z)$$

$$S_- S_+ = S_x^2 + S_y^2 - \hbar S_z$$

Plugging back in, we get

$$\beta^2 = \langle s, m_s | S^2 | s, m_s \rangle - \langle s, m_s | S_z^2 | s, m_s \rangle - \hbar \langle s, m_s | S_z | s, m_s \rangle$$

$$\beta^2 = s(s+1)\hbar^2 \langle s, m_s | s, m_s \rangle - m_s^2 \hbar^2 \langle s, m_s | s, m_s \rangle - m_s \hbar^2 \langle s, m_s | s, m_s \rangle$$

$$\beta^2 = s(s+1)\hbar^2 - m_s^2 \hbar^2 - m_s \hbar^2$$

$$\beta = \sqrt{\hbar^2 (s(s+1) - m_s^2 - m_s)}$$

$$\boxed{\beta = \hbar \sqrt{s(s+1) - m_s(m_s+1)}}$$

Which we can see is the same as what we wanted.

(c) Write down the matricies of $S_\pm$ and use this to find S_x and S_y.

we need to find $S_x = \frac{1}{2}(S_+ + S_-)$
$S_y = \frac{1}{2}(S_+ - S_-)$

we can calculate $S_\pm$ by plugging into the given equation.

$$S_+ = \hbar\sqrt{(3/2)(3/2+1) - (3/2)(3/2+1)}\,|3/2, 3/2+1\rangle$$

$$= \hbar\sqrt{15/4 - 15/4}\,|3/2, 5/2\rangle = 0$$

$$S_+ = \hbar\sqrt{(3/2)(3/2+1) - 1/2(1/2+1)}\,|3/2, 1/2+1\rangle$$

$$= \hbar\sqrt{15/4 - 3/4}\,|3/2, 3/2\rangle$$

$$= \hbar\sqrt{3}\,|3/2, 3/2\rangle$$

$$S_+ = \hbar(2)\,|3/2, 1/2\rangle$$

$$S_+ = \hbar\sqrt{3}\,|3/2, -1/2\rangle$$

Together, we get

$$S_+ = \begin{bmatrix} 0 & \sqrt{3}\hbar & 0 & 0 \\ 0 & 0 & 2\hbar & 0 \\ 0 & 0 & 0 & \sqrt{3}\hbar \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

Doing the same thing with S_- gives us

$$S_- = \hbar\sqrt{(3/2)(3/2+1) - (3/2)(3/2-1)}\, |3/2, 3/2-1\rangle$$

$$= \hbar\sqrt{15/4 - 3/4}\, |3/2, 1/2\rangle$$

$$= \hbar\sqrt{3}\, |3/2, 1/2\rangle$$

$$S_- = \hbar(2)\, |3/2, -1/2\rangle$$

$$S_- = \hbar\sqrt{3}\, |3/2, -3/2\rangle$$

Combining these values together in a matrix gives us

$$S_- = \begin{bmatrix} 0 & 0 & 0 & 0 \\ \sqrt{3}\hbar & 0 & 0 & 0 \\ 0 & 2\hbar & 0 & \sqrt{3} \\ 0 & 0 & \sqrt{3}\hbar & 0 \end{bmatrix}$$

Plugging these into S_x and S_y, we get

$$\boxed{\begin{gathered} S_x = \frac{\hbar}{2}\begin{bmatrix} 0 & \sqrt{3} & 0 & 0 \\ \sqrt{3} & 0 & 2 & 0 \\ 0 & 2 & 0 & \sqrt{3} \\ 0 & 0 & \sqrt{3} & 0 \end{bmatrix} \\ \\ S_y = \frac{\hbar}{2}\begin{bmatrix} 0 & -i\sqrt{3} & 0 & 0 \\ i\sqrt{3} & 0 & -i2 & 0 \\ 0 & i2 & 0 & -i\sqrt{3} \\ 0 & 0 & i\sqrt{3} & 0 \end{bmatrix} \end{gathered}}$$