

# Homework #5 Blake Evans

① Prove the following identity:

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

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

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

So, we can say

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

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

$$\vec{P} \times \vec{L} + \vec{L} \times \vec{P} = [P_y L_z + L_y P_z - P_z L_y - L_z P_y] \hat{x}$$

$$+ [P_x L_y - L_y P_x + P_x L_z - L_x P_z] \hat{y}$$

$$+ [P_x L_y + L_x P_y + P_y L_x - L_y P_x] \hat{z}$$

Now let's simplify

$$\hat{x} : \underbrace{[P_y L_z - L_z P_y]}_{[P_y, L_z]} + \underbrace{[L_y P_z - P_z L_y]}_{[L_y, P_z]}$$

$$\hat{y} : \underbrace{[P_z L_x - L_x P_z]}_{[P_z, L_x]} + \underbrace{[L_z P_x - P_x L_z]}_{[L_z, P_x]}$$

$$\hat{z} : \underbrace{[P_x L_y - L_y P_x]}_{[P_x, L_y]} + \underbrace{[L_x P_y - P_y L_x]}_{[L_x, P_y]}$$

Now let's calculate all the commutators

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

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

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

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

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

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

Plug them all in

$$\begin{aligned} & \left[\hbar^2 \frac{\partial}{\partial x}\right] + \left[\hbar^2 \frac{\partial}{\partial x}\right] + \left[\hbar^2 \frac{\partial}{\partial y}\right] + \left[\hbar^2 \frac{\partial}{\partial y}\right] \\ & + \left[\hbar^2 \frac{\partial}{\partial z}\right] + \left[\hbar^2 \frac{\partial}{\partial z}\right] \\ & = \left(2\hbar^2 \frac{\partial}{\partial x}\right) \hat{x} + \left(2\hbar^2 \frac{\partial}{\partial y}\right) \hat{y} + \left(2\hbar^2 \frac{\partial}{\partial z}\right) \hat{z} \end{aligned}$$

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

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

(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

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

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

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

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

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

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

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

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

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

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

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

$$\hat{x} : \frac{[L_y^2 P_x - P_x L_y^2] + [L_z^2 P_x - P_x L_z^2]}{[L_y^2, P_x] + [L_z^2, P_x]}$$

$$\hat{y} : \frac{[L_x^2 P_y - P_y L_x^2] + [L_z^2 P_y - P_y L_z^2]}{[L_x^2, P_y] + [L_z^2, P_y]}$$

$$\hat{z} : \frac{[L_x^2 P_z - P_z L_x^2] + [L_y^2 P_z - P_z L_y^2]}{[L_x^2, P_z] + [L_y^2, P_z]}$$

$$= [(L_y [L_y, P_x] + [L_y, P_x] L_y)$$

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

$$+ [(L_x [L_x, P_y] + [L_x, P_y] L_x)$$

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

$$+ [(L_x [L_x, P_z] + [L_x, P_z] L_x)$$

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

We can simplify

$$\begin{aligned}x &: \left[ L_y \left( -\hbar^2 \frac{\partial}{\partial z} \right) + \left( -\hbar^2 \frac{\partial}{\partial z} \right) L_y \right] \\&\quad + \left[ L_z \left( \hbar^2 \frac{\partial}{\partial y} \right) + \left( \hbar^2 \frac{\partial}{\partial y} \right) L_z \right] \\&= \left[ -i\hbar (-L_y P_z - P_z L_y) \right] + \left[ i\hbar (L_z P_y + P_y L_z) \right] \\y &: \left[ L_x \left( \hbar^2 \frac{\partial}{\partial x} \right) + \left( \hbar^2 \frac{\partial}{\partial x} \right) L_x \right] \\&\quad + \left[ L_z \left( -\hbar \frac{\partial}{\partial x} \right) + \left( -\hbar \frac{\partial}{\partial x} \right) L_z \right] \\&= \left[ i\hbar (L_x P_z + P_z L_x) \right] + \left[ i\hbar (-L_z P_x - P_x L_z) \right] \\z &: \left[ L_x \left( -\hbar^2 \frac{\partial}{\partial y} \right) + \left( -\hbar^2 \frac{\partial}{\partial y} \right) L_x \right] \\&\quad + \left[ L_y \left( \hbar^2 \frac{\partial}{\partial x} \right) + \left( \hbar^2 \frac{\partial}{\partial x} \right) L_y \right] \\&= \left[ i\hbar (-L_x P_y - P_y L_x) \right] + \left[ i\hbar (L_y P_x - P_x L_y) \right]\end{aligned}$$

Finally, if we combine terms we can see

$$\begin{aligned}
 &= i\hbar [p_y L_z + L_z p_y - L_y p_z - p_z L_y] \hat{x} \\
 &\quad + i\hbar [p_z L_x + L_x p_z - p_x L_z - L_z p_x] \hat{y} \\
 &\quad + i\hbar [p_x L_y + L_y p_x - p_y L_x - L_x p_y] \hat{z}
 \end{aligned}$$

This is the same as what we had before.

$$\begin{aligned}
 \vec{p} \times \vec{L} - \vec{L} \times \vec{p} &= [p_y L_z + L_z p_y - L_y p_z - p_z L_y] \hat{x} \\
 &\quad + [p_z L_x + L_x p_z - p_x L_z - L_z p_x] \hat{y} \\
 &\quad + [p_x L_y + L_y p_x - p_y L_x - L_x p_y] \hat{z}
 \end{aligned}$$

② For a  $\text{CO}_2$  molecule, calculate the first 3 rotational energy levels.

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

where  $B = \frac{\hbar^2}{2I}$  and  $I = \cancel{91} r^2$  reduced mass  
(moment of inertia)

The reduced mass ( $\cancel{91}$ ) of  $\text{CO}_2$  is given by

$$\cancel{91} = \frac{m_c m_o^2}{m_c + 2m_o} = \frac{(12.01 \text{ amu})(15.99 \text{ amu})^2}{(12.01 \text{ amu}) + 2(15.99 \text{ amu})}$$

$$\cancel{91} = 69.8 \text{ amu} \left( \frac{1.66 \times 10^{-27} \text{ kg}}{1 \text{ amu}} \right)$$

$$\cancel{91} = 1.16 \times 10^{-25} \text{ kg}$$

The bond length of  $\text{CO}_2$  is  $r = 116 \times 10^{-12} \text{ m}$

We can put this together to get

$$I = \cancel{91} r^2 = (1.16 \times 10^{-25} \text{ kg}) (116 \times 10^{-12} \text{ m})^2$$

$$I = 1.56 \times 10^{-45} \text{ kg} \cdot \text{m}^2$$

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

$$B = \frac{k^2}{2I} = \frac{(1.054 \times 10^{-34} \text{ J} \cdot \text{s})^2}{2(1.56 \times 10^{-45} \text{ kg} \cdot \text{m}^2)} \quad J = \frac{\text{kg} \cdot \text{m}^2}{\text{s}^2}$$

$$B = 3.56 \times 10^{-24} \text{ J} \left( \frac{\text{kg} \cdot \text{m}^2}{\text{s}^2} \right) \text{s}^2 \left( \frac{1}{\text{kg} \cdot \text{m}^2} \right)$$

$$B = 3.56 \times 10^{-24} \text{ J} \quad \text{or} \quad 2.22 \times 10^{-5} \text{ eV}$$

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

$$E_{(1)} = (2.22 \times 10^{-5} \text{ eV})(1)((1)+1) = 4.44 \times 10^{-5} \text{ eV}$$

$$E_{(2)} = (2.22 \times 10^{-5} \text{ eV})(2)((2)+1) = 1.33 \times 10^{-4} \text{ eV}$$

$$E_{(3)} = (2.22 \times 10^{-5} \text{ eV})(3)((3)+1) = 2.66 \times 10^{-4} \text{ eV}$$

③ Consider a spin- $\frac{3}{2}$  system

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

A spin  $\frac{3}{2}$  system has four possible states:  $\frac{3}{2}, \frac{1}{2}, -\frac{1}{2}, -\frac{3}{2}$ .

The four eigenstates are

$$|sm_s\rangle = |\frac{3}{2}, \frac{3}{2}\rangle, |\frac{3}{2}, \frac{1}{2}\rangle, |\frac{3}{2}, -\frac{1}{2}\rangle, |\frac{3}{2}, -\frac{3}{2}\rangle$$

The eigenvalue equation for  $S^2$  is,

$$S^2 |sm_s\rangle = S(S+1)\hbar^2 |sm_s\rangle = \frac{15}{4}\hbar^2 |\frac{3}{2}, m_s\rangle$$

The eigenvalue equations for  $S_z$  is

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

$$\boxed{S_z |sm_s\rangle = \begin{aligned} & \frac{3}{2}\hbar |\frac{3}{2}, \frac{3}{2}\rangle \\ & \frac{1}{2}\hbar |\frac{3}{2}, \frac{1}{2}\rangle \\ & -\frac{1}{2}\hbar |\frac{3}{2}, -\frac{1}{2}\rangle \\ & -\frac{3}{2}\hbar |\frac{3}{2}, -\frac{3}{2}\rangle \end{aligned}}$$

(b)  $S_{\pm} = S_x \pm iS_y$ . Show that  
 $S_{\pm}|S, M_S\rangle = \hbar \sqrt{S(S+1)-M_S(M_S \pm 1)} |S, M_S \pm 1\rangle$

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

$$\langle S, (M_S+1) | \beta | S, (M_S+1) \rangle = \langle S, M_S | S_- S_+ | S, M_S \rangle$$

$$\beta \cancel{\langle S, (M_S+1) | S, (M_S+1) \rangle}^{\downarrow} = \langle S, M_S | S_- S_+ | S, M_S \rangle$$

Now let's expand  $S_- S_+$ ,

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

$$= S_x^2 + iS_x S_y - iS_y S_x - i^2 S_y^2$$

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

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

$$\langle S, S \rangle = S_x^2 + S_y^2 - \hbar S_z$$

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 matrices 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.

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

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

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

$$= \hbar \sqrt{\frac{15}{4} - \frac{3}{4}} \left| \frac{3}{2}, \frac{3}{2} \right\rangle$$

$$= \hbar \sqrt{3} \left| \frac{3}{2}, \frac{3}{2} \right\rangle$$

$$S_+ = \hbar(2) \left| \frac{3}{2}, \frac{1}{2} \right\rangle$$

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

Together, we get

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

Doing the same thing with  $S_-$  gives us

$$\begin{aligned} S_- &= \hbar \sqrt{(\frac{3}{2})(\frac{3}{2}+1) - (\frac{3}{2})(\frac{3}{2}-1)} | \frac{3}{2}, \frac{3}{2}-1 \rangle \\ &= \hbar \sqrt{\frac{15}{4} - \frac{3}{4}} | \frac{3}{2}, \frac{1}{2} \rangle \\ &= \hbar \sqrt{3} | \frac{3}{2}, \frac{1}{2} \rangle \end{aligned}$$

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

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

Combining these values together in a matrix gives us

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

Plugging these into  $S_x$  and  $S_y$ , we get

$$S_x = \frac{\hbar}{2} \begin{bmatrix} 0 & \sqrt{3} & 0 & 0 \\ \sqrt{3} & 0 & 2 & 0 \\ 0 & 2 & 0 & \sqrt{3} \\ 0 & 0 & \sqrt{3} & 0 \end{bmatrix}$$

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