Quantum Mechanics and Spectroscopy
CHEM 3PA3
Tutorial 6

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1. It is more convenient to express the momentum operators using ladder operators,

$$\hat{M}_+ = \hat{M}_x + i\hat{M}_y \qquad \hat{M}_- = \hat{M}_x - i\hat{M}_y.$$

Here, $\hat{M} = \hat{L}, \hat{S}$, and they give to following eigenvalues for the spherical harmonics,

$$\hat{M}_+ Y_l^m = \hbar\sqrt{l(l+1) - m(m+1)}\, Y_l^{m+1}$$

$$\hat{M}_- Y_l^m = \hbar\sqrt{l(l+1) - m(m-1)}\, Y_l^{m-1}.$$

(a) Express the operators $\hat{M}_x$ and $\hat{M}_y$ in terms of the ladder operators.

(b) Prove that $\hat{M}^2 = \frac{1}{2}\left(\hat{M}_+\hat{M}_- + \hat{M}_-\hat{M}_+\right) + \hat{M}_z^2$.

(c) Show that $[\hat{M}_+, \hat{M}_-] = 2\hbar\hat{M}_z$.

(d) Do the ladder operators commute with the total angular momentum and its individual components?

(e) What does $\hat{M}^2 \left|Y_l^m\right\rangle$ yield?

(f) Calculate the values of the following integrals: (i) $\left\langle p_x \middle| \hat{L}_z \middle| p_y \right\rangle$, (ii) $\left\langle p_x \middle| \hat{L}_+ \middle| p_y \right\rangle$, (iii) $\left\langle p_z \middle| \hat{L}_y \middle| p_x \right\rangle$, (iv) $\left\langle p_z \middle| \hat{L}_x \middle| p_y \right\rangle$, (iiv) $\left\langle p_z \middle| \hat{L}_x \middle| p_x \right\rangle$. Remember that $p_z = p_0$, $p_x = \frac{1}{\sqrt{2}}(p_{-1} - p_{+1})$, and $p_y = \frac{i}{\sqrt{2}}(p_{-1} + p_{+1})$.

② $M_+ = \hat{M}_x + i\hat{M}_y \quad \rightarrow \quad \hat{M}_+ Y_\ell^m = \hbar\sqrt{\ell(\ell+1)-m(m+1)}\, Y_\ell^{m+1}$

$M_- = \hat{M}_x - i\hat{M}_y \quad \rightarrow \quad \hat{M}_- Y_\ell^m = \hbar\sqrt{\ell(\ell+1)-m(m-1)}\, Y_\ell^{m-1}$

a) $\hat{M}_x = \dfrac{\hat{M}_+ + \hat{M}_-}{2}$; $\hat{M}_y = \dfrac{\hat{M}_+ - \hat{M}_-}{2i}$

b) $\hat{M}^2 = \frac{1}{2}(\hat{M}_+\hat{M}_- + \hat{M}_-\hat{M}_+) + \hat{M}_z^2$

$\hat{M}_x^2 + \hat{M}_y^2 + \cancel{\hat{M}_z^2} = \frac{1}{2}(\hat{M}_+\hat{M}_- + \hat{M}_-\hat{M}_+) + \cancel{\hat{M}_z^2}$

$\left(\dfrac{\hat{M}_+ + \hat{M}_-}{2}\right)^2 + \left(\dfrac{\hat{M}_+ - \hat{M}_-}{2i}\right)^2 = \frac{1}{2}(\hat{M}_+\hat{M}_- + \hat{M}_-\hat{M}_+)$

$\dfrac{\hat{M}_+\hat{M}_+ + \hat{M}_+\hat{M}_- + \hat{M}_-\hat{M}_+ + \hat{M}_-\hat{M}_-}{4} + \dfrac{\hat{M}_+\hat{M}_+ - \hat{M}_+\hat{M}_- - \hat{M}_-\hat{M}_+ + \hat{M}_-\hat{M}_-}{4(-1)} = \frac{1}{2}(\hat{M}_+\hat{M}_- + \hat{M}_-\hat{M}_+)$

$\dfrac{\hat{M}_+\hat{M}_+ + \hat{M}_+\hat{M}_- + \hat{M}_-\hat{M}_+ + \hat{M}_-\hat{M}_- - \hat{M}_+\hat{M}_+ + \hat{M}_+\hat{M}_- + \hat{M}_-\hat{M}_+ - \hat{M}_-\hat{M}_-}{4} = \frac{1}{2}(\hat{M}_+\hat{M}_- + \hat{M}_-\hat{M}_+)$

$\frac{1}{2}(\hat{M}_+\hat{M}_- + \hat{M}_-\hat{M}_+) = \frac{1}{2}(\hat{M}_+\hat{M}_- + \hat{M}_-M_+)$ ✓

c) $[\hat{M}_+, \hat{M}_-] = 2\hbar\hat{M}_z$

$\hat{M}_+\hat{M}_- - \hat{M}_-\hat{M}_+ = 2\hbar\hat{M}_z$

$[\hat{M}_+\hat{M}_- - \hat{M}_-\hat{M}_+]Y_\ell^m = \hat{M}_+\left[\hbar\sqrt{\ell(\ell+1)-m(m-1)}\, Y_\ell^{m-1}\right] - \hat{M}_-\left[\hbar\sqrt{\ell(\ell+1)-m(m+1)}\, Y_\ell^{m+1}\right]$

$= \hbar^2\sqrt{\ell(\ell+1)-m(m-1)}\sqrt{\ell(\ell+1)-(m-1)m}\, Y_\ell^m - \hbar^2\sqrt{\ell(\ell+1)-m(m+1)}\sqrt{\ell(\ell+1)-(m+1)m}\, Y_\ell^m$

$= \hbar^2[\cancel{\ell(\ell+1)} - m(m-1) - \cancel{\ell(\ell+1)} + m(m+1)]Y_\ell^m$

$= \hbar^2[\cancel{m^2} + m - \cancel{m^2} + m]Y_\ell^m = 2\hbar^2 m Y_\ell^m = 2\hbar\hat{M}_z Y_\ell^m$

d) $[\hat{M}_+, \hat{M}_x] = [\hat{M}_x + i\hat{M}_y, \hat{M}_x] = [\hat{M}_x, \hat{M}_x] + i[\hat{M}_y, \hat{M}_x] = 0 + i[-i\hbar\hat{M}_z] = \hbar\hat{M}_z$

$[\hat{M}_+, \hat{M}_y] = [\hat{M}_x + i\hat{M}_y, \hat{M}_y] = [\hat{M}_x, \hat{M}_y] + 0i = i\hbar\hat{M}_z$

$[\hat{M}_+, \hat{M}_z] = [\hat{M}_x + i\hat{M}_y, \hat{M}_z] = [\hat{M}_x, \hat{M}_z] + i[\hat{M}_y, \hat{M}_z] = -i\hbar\hat{M}_y + i[i\hbar\hat{M}_x] = -\hbar[\hat{M}_x + i\hat{M}_y]$

$= -\hbar\hat{M}_+$

$[M^2, M_+] = [M_x^2 + M_y^2 + M_z^2, M_+] = [\hat{M}_x^2, M_+] + [M_y^2, M_+] + [M_z^2, M_+]$

$= \hat{M}_x[\hat{M}_x, M_+] + [\hat{M}_x, \hat{M}_+]\hat{M}_x + \hat{M}_y[\hat{M}_y, \hat{M}_+] + [\hat{M}_y, \hat{M}_+]\hat{M}_y + \hat{M}_z[\hat{M}_z, \hat{M}_+] + [\hat{M}_z, \hat{M}_+]\hat{M}_z$

$= \hat{M}_x(-\hbar\hat{M}_z) + (-\hbar\hat{M}_z)\hat{M}_x + \hat{M}_y(-i\hbar\hat{M}_z) + (-i\hbar\hat{M}_z)\hat{M}_y + \hat{M}_z(\hbar\hat{M}_+) + (\hbar\hat{M}_+)\hat{M}_z$

$= -\hbar[\hat{M}_x, \hat{M}_z] - i\hbar[\hat{M}_y, \hat{M}_z] + \hbar[\hat{M}_z, \hat{M}_+]$

$= -\hbar[-i\hbar\hat{M}_y] - i\hbar[i\hbar\hat{M}_x] + \hbar[\hbar\hat{M}_+] = \hbar^2\hat{M}_x + i\hbar^2\hat{M}_y - \hbar^2[\hat{M}_x + i\hat{M}_y] = 0$

only $[M^2, M_\pm] = 0$

e) $\hat{L}^2 |Y_\ell^m\rangle = \ell(\ell+1)\hbar^2 |Y_\ell^m\rangle$

f) i) $\langle p_x|\hat{L}_z|p_y\rangle = \langle \frac{1}{\sqrt{2}}(p_{-1}-p_{+1})|\hat{L}_z|\frac{i}{\sqrt{2}}(p_{-1}+p_{+1})\rangle = \frac{i}{2}\langle p_{-1}-p_{+1}|\hat{L}_z p_{-1}+\hat{L}_z p_{+1}\rangle$

$= \frac{i}{2}\langle p_{-1}-p_{+1}|\hbar(-1)p_{-1}+\hbar(+1)p_{+1}\rangle = \frac{i\hbar}{2}\langle p_{-1}-p_{+1}|p_{+1}-p_{-1}\rangle$

$= \frac{i\hbar}{2}[\langle p_{-1}|p_{+1}\rangle^{0} - \langle p_{-1}|p_{-1}\rangle^{1} - \langle p_{+1}|p_{+1}\rangle^{1} + \langle p_{+1}|p_{-1}\rangle^{0}] = \frac{i\hbar}{2}[-1-1] = -i\hbar$

ii) $\langle p_x|\hat{L}_+|p_y\rangle = \langle\frac{1}{\sqrt{2}}(p_{-1}-p_{+1})|\hat{L}_+|\frac{i}{\sqrt{2}}(p_{-1}+p_{+1})\rangle = \frac{i}{2}\langle p_{-1}-p_{+1}|\hat{L}_+p_{-1}+\hat{L}_+p_{+1}\rangle$

$= \frac{i}{2}\langle p_{-1}-p_{+1}|\hbar\sqrt{1(1+1)-(-1)(0)}\,p_0 + \hbar\sqrt{1(1+1)-(1)(1+1)}\,(p_{+2})\rangle$ cannot happen and square root is 0

$= \frac{i}{2}\langle p_{-1}-p_{+1}|\hbar\sqrt{2}\,p_0\rangle = \frac{i\hbar}{\sqrt{2}}[\langle p_{-1}|p_0\rangle^{0} - \langle p_{+1}|p_0\rangle^{0}] = 0$

iii) $\langle p_z|\hat{L}_y|p_x\rangle = \langle p_0|\hat{L}_y|\frac{1}{\sqrt{2}}(p_{-1}-p_{+1})\rangle = \langle p_0|\frac{1}{\sqrt{2}}(\hat{L}_y p_{-1}-\hat{L}_y p_{+1})\rangle$

$= \frac{1}{\sqrt{2}}\langle p_0|(\hat{L}_+-\hat{L}_-)(\frac{1}{2i})p_{-1} + (\hat{L}_- - \hat{L}_+)(\frac{1}{2i})p_{+1}\rangle$

$= \frac{\hbar}{2i\sqrt{2}}\langle p_0|\sqrt{1(1+1)-(-1)(0)}\,p_0 - \sqrt{1(1+1)-(-1)(-1-1)}\,(p_{-2})$ cannot happen $+ \sqrt{1(1+1)-1(1-1)}\,p_0 - \sqrt{1(1+1)-(1)(1+1)}\,(p_{+2})\rangle$ cannot happen

$= \frac{\hbar}{2i\sqrt{2}}\langle p_0|\sqrt{2}\,p_0+\sqrt{2}\,p_0\rangle = -\frac{\hbar}{2i}(2)\langle p_0|p_0\rangle = i\hbar$

iv) $\langle p_z|\hat{L}_x|p_y\rangle = \langle p_0|\hat{L}_x|\frac{i}{\sqrt{2}}(p_{-1}+p_{+1})\rangle = \frac{i}{\sqrt{2}}\langle p_0|\hat{L}_x(p_{-1}+p_{+1})\rangle$

$= \frac{i}{\sqrt{2}}\langle p_0|(\hat{L}_+ + \hat{L}_-)p_{-1} + (\hat{L}_+ + \hat{L}_-)p_{+1}\rangle(\frac{1}{2})$

$= \frac{i\hbar}{2\sqrt{2}}\langle p_0|\sqrt{1(1+1)-(-1)(-1+1)}\,p_0 + 0 + 0 + \sqrt{1(2)-(1)(0)}\,p_0\rangle = \frac{i\hbar}{2\sqrt{2}}\langle p_0|\sqrt{2}\,p_0+\sqrt{2}\,p_0\rangle$

$= \frac{i\hbar}{2}\langle p_0|p_0\rangle(2) = i\hbar$

v) $\langle p_z|\hat{L}_x|p_x\rangle = \langle p_0|\hat{L}_x|\frac{1}{\sqrt{2}}(p_{-1}-p_{+1})\rangle = \frac{1}{\sqrt{2}}\langle p_0|\hat{L}_x p_{-1} - \hat{L}_x p_{+1}\rangle = \frac{1}{\sqrt{2}}\langle p_0|(\hat{L}_+ + \hat{L}_-)(\frac{1}{2})p_{-1} - \frac{1}{2}(\hat{L}_+ + \hat{L}_-)p_{+1}\rangle$

$= \frac{\hbar}{2\sqrt{2}}\langle p_0|\sqrt{1(2)-(-1)(0)}\,p_0 + 0 - 0 + \sqrt{1(2)-(1)(0)}\,p_0\rangle = \frac{\hbar}{2\sqrt{2}}\langle p_0|\sqrt{2}\,p_0+\sqrt{2}\,p_0\rangle = \hbar$