## Angular Momentum Matrix Elements

LAST TIME: * all [, ]=0 Commutation Rules needed to block diagonalize

$$\mathbf{H} = \frac{\mathbf{p}_r^{\;2}}{2\mu} + \left[\frac{\mathbf{L}^2}{2\mu\mathbf{r}^2} + V(\mathbf{r})\right] \text{ in } |\mathrm{nLM_L}\rangle \text{ basis set}$$

* $\varepsilon_{ijk}$ Levi-Civita antisymmetric tensor — useful properties

* Commutation Rule DEFINITIONS of Angular Momentum and "Vector" Operators $\left[\mathbf{L}_i, \mathbf{L}_j\right] = i\hbar\sum_k \varepsilon_{ijk}\mathbf{L}_k$

$$\left[\mathbf{L}_i, \mathbf{V}_j\right] = i\hbar\sum_k \varepsilon_{ijk}\mathbf{V}_k$$

Classification of operators: universality of matrix elements.

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TODAY: Obtain <u>all</u> angular momentum matrix elements from the commutation rule definition of an angular momentum, without ever looking at a differential operator or a wavefuncton. *Possibilities for phase inconsistencies.* [Similar derivation for angular parts of matrix elements of all spherical tensor operators, $\mathbf{T}_q^{(k)}$.]

1. Define Components of Angular Momentum using a Commutation Rule.

2. Define eigenbasis for $J^2$ and $J_z$ $|\lambda\mu\rangle$

3. show $\lambda \geq \mu^2$

4 raising and lowering operators (like $\mathbf{a}^\dagger$, $\mathbf{a}$ and $\tilde{\mathbf{x}} \pm i\tilde{\mathbf{p}}$)

   $\mathbf{J}_\pm|\lambda\mu\rangle$ gives eigenfunction of $\mathbf{J}_z$ belonging to $\mu \pm \hbar$ eigenvalue and eigenfunction of $\mathbf{J}^2$ belonging to $\lambda$ eigenvalue

5. Must be at least one $\mu_{MAX}$ and one $\mu_{MIN}$ such that

   $\mathbf{J}_-(\mathbf{J}_+|\lambda\mu_{MAX}\rangle) = 0$

   $\mathbf{J}_+(\mathbf{J}_-|\lambda\mu_{MIN}\rangle) = 0$

   This leads to $\mu_{max} = \hbar\left(\frac{n}{2}\right), \lambda = \hbar^2\frac{n}{2}\left(\frac{n}{2}+1\right)$.

6. Obtain all matrix elements of $\mathbf{J}_x$, $\mathbf{J}_y$, $\mathbf{J}_\pm$, but there remains a phase ambiguity

7. Standard phase choice: "Condon and Shortley"

1. Commutation Rule $\left[J_i, J_j\right] = i\hbar\sum_k \varepsilon_{ijk} J_k$
   *This is a general definition of angular momentum* (call it **J**, **L**, **S**, anything!). Each angular momentum generates a state space.

2. eigenfunctions of $\mathbf{J}^2$ and $\mathbf{J}_z$ exist (Hermitian operators. Guaranteed by symmetrization.)

$$\mathbf{J}^2|\lambda\mu\rangle = \lambda|\lambda\mu\rangle$$
$$\mathbf{J}_z|\lambda\mu\rangle = \mu|\lambda\mu\rangle$$

but what are the values of $\lambda,\mu$?

$\mathbf{J}^2$ and $\mathbf{J}_z$ are Hermitian, therefore $\lambda,\mu$ are real

3. find upper and lower bounds for $\mu$ in terms of $\lambda : \lambda \geq \mu^2$

$$\langle\lambda\mu|(\mathbf{J}^2 - \mathbf{J}_z^2)|\lambda\mu\rangle = \lambda - \mu^2$$ Want to show that this is $\geq 0$.

but $\mathbf{J}^2 = \mathbf{J}_x^2 + \mathbf{J}_y^2 + \mathbf{J}_z^2$

$$\mathbf{J}^2 - \mathbf{J}_z^2 = \mathbf{J}_x^2 + \mathbf{J}_y^2$$

$$\lambda - \mu^2 = \langle\lambda\mu|\mathbf{J}_x^2 + \mathbf{J}_y^2|\lambda\mu\rangle$$

completeness

$$\lambda - \mu^2 = \sum_{\lambda',\mu'} \left[\langle\lambda\mu|\mathbf{J}_x|\lambda'\mu'\rangle\langle\lambda'\mu'|\mathbf{J}_x|\lambda\mu\rangle + \langle\lambda\mu|\mathbf{J}_y|\lambda'\mu'\rangle\langle\lambda'\mu'|\mathbf{J}_y|\lambda\mu\rangle\right]$$

Hermitian: $\langle\lambda'\mu'|\mathbf{J}_x|\lambda\mu\rangle = \langle\lambda\mu|\mathbf{J}_x|\lambda'\mu'\rangle^*$

$$\lambda - \mu^2 = \sum_{\lambda',\mu'} \left[\left|\langle\lambda\mu|\mathbf{J}_x|\lambda'\mu'\rangle\right|^2 + \left|\langle\lambda\mu|\mathbf{J}_y|\lambda'\mu'\rangle\right|^2\right] \geq 0$$

Thus $\lambda - \mu^2 \geq 0$ and $\lambda \geq \mu^2 \geq 0$

and $\mu_{MAX} \leq \lambda^{1/2}$, $\mu_{MIN} \geq -\lambda^{1/2}$

4. Raising/Lowering Operators

$$\mathbf{J}_{\pm} \equiv \mathbf{J}_x \pm i\mathbf{J}_y \quad \left(\text{not Hermitian: } \mathbf{J}_+^\dagger = \mathbf{J}_-\right) \qquad \left(\text{just like } \mathbf{a},\mathbf{a}^\dagger\right)$$

$$\begin{aligned}[\mathbf{J}_z,\mathbf{J}_\pm] &= [\mathbf{J}_z,\mathbf{J}_x] \pm i[\mathbf{J}_z,\mathbf{J}_y] \\ &= i\hbar\mathbf{J}_y \pm i(-i\hbar\mathbf{J}_x) = \pm\hbar[\mathbf{J}_x \pm i\mathbf{J}_y] \\ &= \pm\hbar\mathbf{J}_\pm\end{aligned}$$

$$\mathbf{J}_z\mathbf{J}_\pm = \mathbf{J}_\pm\mathbf{J}_z \pm \hbar\mathbf{J}_\pm \qquad \text{right multiply by } |\lambda\mu\rangle$$

$$\begin{aligned}\mathbf{J}_z\left(\mathbf{J}_\pm|\lambda\mu\rangle\right) &= \mathbf{J}_\pm\left(\mathbf{J}_z|\lambda\mu\rangle\right) \pm \hbar\mathbf{J}_\pm|\lambda\mu\rangle \\ &= \mathbf{J}_\pm\mu|\lambda\mu\rangle \pm \hbar\mathbf{J}_\pm|\lambda\mu\rangle \\ &= (\mu \pm \hbar)\left(\mathbf{J}_\pm|\lambda\mu\rangle\right)\end{aligned}$$

$\left(\mathbf{J}_\pm|\lambda\mu\rangle\right)$ is an eigenfunction of $\mathbf{J}_z$ belonging to eigenvalue $\mu \pm \hbar$.

Thus $\mathbf{J}_\pm$ "raises" or "lowers" $\mathbf{J}_z$ eigenvalue in steps of $\hbar$.

Similar exercise for $\left[\mathbf{J}^2,\mathbf{J}_\pm\right]$ to get effect of $\mathbf{J}_\pm$ on eigenvalue of $\mathbf{J}^2$

$\left[\mathbf{J}^2,\mathbf{J}_\pm\right] = \left[\mathbf{J}^2,\mathbf{J}_x\right] \pm i\left[\mathbf{J}^2,\mathbf{J}_y\right] = 0 \quad$ (We already know that $\left[\mathbf{J}^2,\mathbf{J}_i\right] = 0$)

$\mathbf{J}^2\left(\mathbf{J}_\pm|\lambda\mu\rangle\right) = \mathbf{J}_\pm\left(\mathbf{J}^2|\lambda\mu\rangle\right) = \lambda\left(\mathbf{J}_\pm|\lambda\mu\rangle\right)$

$\left(\mathbf{J}_\pm|\lambda\mu\rangle\right)$ belongs to same eigenvalue of $\mathbf{J}^2$ as $|\lambda\mu\rangle$

$\mathbf{J}_\pm$ has no effect on $\lambda$.

* upper and lower bounds on $\mu$ are $\pm\lambda^{1/2}$

* $\mathbf{J}_{\pm}$ raises/lowers $\mu$ by steps of $\hbar$

* Since $\mathbf{J}_x = \frac{1}{2}(\mathbf{J}_+ + \mathbf{J}_-)$ and $\mathbf{J}_y = \frac{1}{2i}(\mathbf{J}_+ - \mathbf{J}_-)$,

The only nonzero matrix elements of $\mathbf{J}_i$ in the $|\lambda\mu\rangle$ basis set are those where $\Delta\mu = 0, \pm\hbar$ and $\Delta\lambda = 0$. As for derivation of Harmonic Oscillator matrix elements, we are not assured that all $\mu$ differ in steps of $\hbar$. Divide basis states into sets related by integer steps of $\hbar$ in $\mu$.

5. For each set, there are $\mu_{\text{MIN}}$ and $\mu_{\text{MAX}}$: $\lambda \ge \mu^2$

Thus, for each set
$$\mathbf{J}_+|\lambda\mu_{\text{MAX}}\rangle = 0$$
$$\mathbf{J}_-|\lambda\mu_{\text{MIN}}\rangle = 0$$

but
$$\begin{aligned}\mathbf{J}_-\mathbf{J}_+ = (\mathbf{J}_x - i\mathbf{J}_y)(\mathbf{J}_x + i\mathbf{J}_y) &= \mathbf{J}_x^2 + \mathbf{J}_y^2 + i\mathbf{J}_x\mathbf{J}_y - i\mathbf{J}_y\mathbf{J}_x \\ &= \mathbf{J}_x^2 + \mathbf{J}_y^2 + i[\mathbf{J}_x, \mathbf{J}_y] \\ &= \mathbf{J}_x^2 + \mathbf{J}_y^2 + i(i\hbar\mathbf{J}_z) \\ &= \mathbf{J}_x^2 + \mathbf{J}_y^2 - \hbar\mathbf{J}_z\end{aligned}$$

but $\mathbf{J}_x^2 + \mathbf{J}_y^2 = \mathbf{J}^2 - \mathbf{J}_z^2$, thus
$$\mathbf{J}_-\mathbf{J}_+ = \mathbf{J}^2 - \mathbf{J}_z^2 - \hbar\mathbf{J}_z$$

$$\begin{aligned}0 = \mathbf{J}_-\mathbf{J}_+|\lambda\mu_{\text{MAX}}\rangle &= (\mathbf{J}^2 - \mathbf{J}_z^2 - \hbar\mathbf{J}_z)|\lambda\mu_{\text{MAX}}\rangle \\ &= (\lambda - \mu_{\text{MAX}}^2 - \hbar\mu_{\text{MAX}})|\lambda\mu_{\text{MAX}}\rangle\end{aligned}$$

$$\lambda = \mu_{\text{MAX}}^2 + \hbar\mu_{\text{MAX}}$$

Similarly for $\mu_{\text{MIN}}$
$$\mathbf{J}_+\mathbf{J}_-|\lambda\mu_{\text{MIN}}\rangle = 0$$

$$\mathbf{J}_+\mathbf{J}_- = \mathbf{J}^2 - \mathbf{J}_z^2 + \hbar\mathbf{J}_z$$

$$\lambda = \mu_{\text{MIN}}^2 - \hbar\mu_{\text{MIN}}$$

subtract 2 equations for $\lambda$

$$0 = \mu_{\text{MAX}}^2 - \mu_{\text{MIN}}^2 + \hbar(\mu_{\text{MAX}} + \mu_{\text{MIN}})$$

$$0 = (\mu_{\text{MAX}} + \mu_{\text{MIN}})(\mu_{\text{MAX}} - \mu_{\text{MIN}} + \hbar)$$

now factor this equation

Thus $\mu_{\text{MAX}} = -\mu_{\text{MIN}}$ OR $\mu_{\text{MAX}} = \mu_{\text{MIN}} - \hbar$ *(impossible)*

Thus for each set of $|\lambda\mu\rangle$, $\mu$ goes from $\mu_{\text{MAX}}$ to $\mu_{\text{MIN}}$ in steps of $\hbar$

$$\mu_{\text{MAX}} = \mu_{\text{MIN}} + n\hbar = -\mu_{\text{MAX}} + n\hbar$$

$$\mu_{\text{MAX}} = \frac{n}{2}\hbar$$

Thus $\mu$ is either integer or half integer or both!

Thus there will at worst be only two non-communicating sets of $|\lambda\mu\rangle$ because if $\mu$ were both integer and 1/2-integer, each would form a set of $\mu$-values, the members of which would be separated in steps of $\hbar$.

Now, to specify allowed values of $\lambda$:

$$\lambda = \mu_{\text{MAX}}^2 + \hbar\mu_{\text{MAX}} = \left(\frac{n}{2}\hbar\right)^2 + \hbar\left(\frac{n}{2}\hbar\right) = \hbar^2\frac{n}{2}\left(\frac{n}{2}+1\right)$$

let $\frac{n}{2} \equiv j$

$$\mu_{\text{MAX}} = \hbar j$$
$$\mu_{\text{MIN}} = -\hbar j$$
$$\lambda = \hbar^2 j(j+1)$$

!

j either integer or half integer or both rename our basis states

$$\mathbf{J}^2|jm\rangle = \hbar^2 j(j+1)|jm\rangle$$
$$\mathbf{J}_z|jm\rangle = \hbar m|jm\rangle$$

valid for all operators that satisfy $[\mathbf{A}_i,\mathbf{A}_j] = i\hbar\sum_k \varepsilon_{ijk}\mathbf{A}_k$

OK to define an $|am_a\rangle$ basis set for any angular momentum operator defined as above.

6. <u>$\mathbf{J}_x$, $\mathbf{J}_y$, $\mathbf{J}_\pm$ matrix elements</u>

recall page 23-3, but in new notation

$$|jm\pm 1\rangle = N_\pm \mathbf{J}_\pm |jm\rangle \qquad (\mathbf{J}_\pm \text{ raises / lowers } m \text{ by } 1)$$

$N_\pm$: normalization factor (to be determined below)

$$1 = \langle jm\pm 1|jm\pm 1\rangle = \left(N_\pm \mathbf{J}_\pm|jm\rangle\right)^\dagger \left(N_\pm \mathbf{J}_\pm |jm\rangle\right)$$
$$N_\pm^\dagger = N_\pm^*$$
$$\mathbf{J}_\pm^\dagger = \mathbf{J}_\mp \qquad !$$

$$1 = |N_\pm|^2 \langle jm|\mathbf{J}_\mp \mathbf{J}_\pm|jm\rangle$$

$$\mathbf{J}_\mp\mathbf{J}_\pm = (\mathbf{J}_x \mp i\mathbf{J}_y)(\mathbf{J}_x \pm i\mathbf{J}_y) = \mathbf{J}_x^2 + \mathbf{J}_y^2 \pm i[\mathbf{J}_x,\mathbf{J}_y]$$
$$= \mathbf{J}^2 - \mathbf{J}_z^2 \pm i(i\hbar \mathbf{J}_z) = \mathbf{J}^2 - \mathbf{J}_z^2 \mp \hbar \mathbf{J}_z$$
$$= \mathbf{J}^2 - \mathbf{J}_z(\mathbf{J}_z \pm \hbar)$$

use this to evaluate matrix elements of $\mathbf{J}_\mp\mathbf{J}_\pm$

$$1 = |N_\pm|^2\left[\hbar^2 j(j+1) - \hbar^2(m(m\pm 1))\right]$$

$$|N_\pm| = \frac{1}{\hbar}\left[j(j+1) - m(m\pm 1)\right]^{-1/2} \underbrace{e^{-i\delta_\pm}}$$

($e^{-i\delta_\pm}$: arbitrary phase factor from taking square root)

$$\mathbf{J}_\pm|jm\rangle = \hbar\left[j(j+1) - m(m\pm 1)\right]^{1/2} |jm\pm 1\rangle e^{-i\delta_\pm}$$

Usual phase choice is $\delta_\pm = 0$ for all j,m:
the "Condon and Shortley" phase choice
(sometimes $\delta_\pm = \pm\pi/2$ – so be careful)

std. phase choice: $\delta_{\pm} = 0$

$$\left\langle j'm' \middle| \mathbf{J}_{\pm} \middle| jm \right\rangle = \hbar \delta_{j'j} \delta_{m' m\pm 1} \left[ j(j+1) - m(m \pm 1) \right]^{1/2}$$

$$\left( \text{or } \hbar \delta_{jj'} \delta_{m' m\pm 1} \left[ j(j+1) - \underline{\underline{m(m')}} \right]^{1/2} \right)$$

remember matrix elements of **x** and **p** in harmonic oscillator basis set?

since $\mathbf{J}_x = \frac{1}{2}(\mathbf{J}_+ + \mathbf{J}_-)$

$$\left\langle j'm' \middle| \mathbf{J}_x \middle| jm \right\rangle = \frac{\hbar}{2} \delta_{j'j} \left\{ \delta_{m' m+1} \left[ j(j+1) - m(m+1) \right]^{1/2} + \delta_{m' m-1} \left[ j(j+1) - m(m-1) \right]^{1/2} \right\}$$

$\mathbf{J}_y = \frac{1}{2i}(\mathbf{J}_+ - \mathbf{J}_-)$

$$\left\langle j'm' \middle| \mathbf{J}_y \middle| jm \right\rangle = -i \frac{\hbar}{2} \delta_{j'j} \left\{ \delta_{m' m+1} \left[ j(j+1) - m(m+1) \right]^{1/2} - \delta_{m' m-1} \left[ j(j+1) - m(m-1) \right]^{1/2} \right\}$$

two sign surprises

This phase choice leaves all matrix elements of $\mathbf{J}^2, \mathbf{J}_x$ and $\mathbf{J}_{\pm}$ real and positive, but those of $\mathbf{J}_y$ imaginary

[if use $\delta_{\pm} = +\pi/2$, this gives $\mathbf{J}_y$ real and $\mathbf{J}_x, \mathbf{J}_{\pm}$ imaginary]

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Summary

$$\left\langle j'm' \middle| \mathbf{J}^2 \middle| jm \right\rangle = \delta_{j'j} \delta_{m'm} \hbar^2 j(j+1)$$

$$\left\langle jm \middle| \vec{\mathbf{J}} \middle| jm \right\rangle = \hat{k} \hbar m$$

$$\left\langle jm \pm 1 \middle| \vec{\mathbf{J}} \middle| jm \right\rangle = \left( \hat{i} \mp i\hat{j} \right) \frac{\hbar}{2} \left[ j(j+1) - m(m \pm 1) \right]^{1/2}$$

$$\hat{i}\mathbf{J}_x + \hat{j}\mathbf{J}_y = \frac{1}{2} \hat{i} (\mathbf{J}_+ + \mathbf{J}_-) + \hat{j} \frac{1}{2i} (\mathbf{J}_+ - \mathbf{J}_-)$$

$$= \frac{1}{2} \mathbf{J}_+ \left( \hat{i} - i\hat{j} \right) + \frac{1}{2} \mathbf{J}_- \left( \hat{i} + i\hat{j} \right)$$