Angular Momentum Matrix Elements Derived from Commutation Rules

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

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

*ε_{ijk} Levi-Civita antisymmetric tensor — useful properties, especially for derivations involving components of angular momenta

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

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

Classification of operators: *universality* of angular factors of matrix elements for 3D central force problems.

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 generalization to derivation for angular parts of matrix elements of all "spherical tensor" operators, $\mathbf{T}_q^{(k)}$.]

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

2. Define the eigenbasis for J^2 and J_z. $|\lambda\mu\rangle$ (we know the eigenbasis must exist, but we start out not knowing anything about it).

3. Show $\lambda \geq \mu$.

4. Raising and lowering operators (like $\mathbf{a}^\dagger$, $\mathbf{a}$ and $\boldsymbol{x} \pm i\boldsymbol{p}$ for the harmonic oscillator). $\mathbf{J}_\pm|\lambda\mu\rangle$ gives eigenfunction of $\mathbf{J}_z$ that belongs to the $\mu \pm \hbar$ eigenvalue and the eigenfuncton of $\mathbf{J}^2$ that belongs to the λ eigenvalue.

5. Must be at least one μ_{MIN} pair of eigenstates of $\mathbf{J}_z$ such that

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

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

   This leads to: $\hbar\left(\frac{n}{2}\right), \lambda = \hbar^2 \frac{n}{2}\left(\frac{n}{2} + 1\right)$, and n is a positive integer.

6. Obtain all matrix elements of $\mathbf{J}_x$, $\mathbf{J}_y$, $\mathbf{J}_\pm$, but there remains. phase ambiguity for the non-zero matrix elements.

7. Standard phase choice: "Condon and Shortley".

1. Commutation Rule $\left[\mathrm{J}_i,\mathrm{J}_j\right]=i\hbar\sum_k \varepsilon_{ijk}\mathrm{J}_k$
   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. Hermiticity is 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 λ,μ?
$\mathbf{J}^2$ and $\mathbf{J}_z$ are Hermitian, therefore λ,μ are real

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

$$\left\langle\lambda\mu\middle|(\mathbf{J}^2-\mathbf{J}_z^2)\middle|\lambda\mu\right\rangle=\lambda-\mu^2$$

Want to show that $\lambda-\mu^2$ is ≥ 0.

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

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

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

completeness

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

We know that $\mathbf{J}^2$ and $\mathbf{J}_z$ are Hermitian because they were constructed by symmetrization of classical mechanical operators.

Hermitian ($\mathbf{A}=\mathbf{A}^\dagger$ or $A_{ij}=A_{ji}^*$): $\left\langle\lambda'\mu'\middle|\mathbf{J}_x\middle|\lambda\mu\right\rangle=\left\langle\lambda\mu\middle|\mathbf{J}_x\middle|\lambda'\mu'\right\rangle^*$

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

Thus $\lambda-\mu^2\geq 0$ and $\lambda\geq\mu^2\geq 0$
and from these we get $\mu_{\mathrm{MAX}}\leq\lambda^{1/2},\mu_{\mathrm{MIN}}\geq-\lambda^{1/2}$

4. Raising/Lowering Operators

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

$$\left[\mathbf{J}_z,\mathbf{J}_{\pm}\right] = \left[\mathbf{J}_z,\mathbf{J}_x\right] \pm i\left[\mathbf{J}_z,\mathbf{J}_y\right]$$

$$= i\hbar\mathbf{J}_y \pm i\left(-i\hbar\mathbf{J}_x\right) = \pm\hbar\left[\mathbf{J}_x \pm i\mathbf{J}_y\right]$$

$$= \pm\hbar\mathbf{J}_{\pm}$$

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

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

$$= \mathbf{J}_{\pm}\mu|\lambda\mu\rangle \pm \hbar\mathbf{J}_{\pm}|\lambda\mu\rangle$$

$$= \left(\mu \pm \hbar\right)\left(\mathbf{J}_{\pm}|\lambda\mu\rangle\right), \text{ which means that}$$

($\mathbf{J}_{\pm}|\lambda\mu\rangle$) is an eigenfunction of $\mathbf{J}_z$ belonging to eigenvalue $\mu \pm \hbar$. Thus $\mathbf{J}_{\pm}$ "raises" or "lowers" the $\mathbf{J}_z$ 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 $\mathbf{J}^2$

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

$$\mathbf{J}^2\left(\mathbf{J}_{\pm}|\lambda\mu\rangle\right) = \mathbf{J}_{\pm}\left(\mathbf{J}^2|\lambda\mu\rangle\right) = \lambda\left(\mathbf{J}_{\pm}|\lambda\mu\rangle\right), \text{ which means that}$$

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

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

* upper and lower bounds on μ are $\pm\lambda^{1/2}$
* $\mathbf{J}_{\pm}$ raises/lowers μ 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* values of μ differ in steps of $\hbar$. Divide basis states into sets, where the members of each set are related by integer steps of $\hbar$ in μ.

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

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

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

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

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

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

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

Similarly for μ_{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 λ

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

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

now factor this equation

Thus $\mu_{\text{MAX}} = -\mu_{\text{MIN}}$ OR $\mu_{\text{MAX}} = \mu_{\text{MIN}} - \hbar$

(*impossible* because μ_{MAX} cannot be smaller than μ_{MIN})

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

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

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

Thus μ 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 μ were both integer and 1/2-integer, each set would form a set of μ-values, within which the members would be separated in steps of $\hbar$.

Now, to specify the allowed values of λ:

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

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

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

!

j either integer or half integer or both

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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 angular momentum operators that are certified as an angular momentum by satisfying the defining commutation rule $\left[A_i, A_j\right] = i\hbar\sum_k \varepsilon_{ijk} A_k$. We can define an $|am_a\rangle$ basis set for any angular momentum operator defined as above. We never need to look at the functional form of the $\{\psi_{am_a}\}$ wavefunctions!

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)

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

$$N_\pm^\dagger = N_\pm^*$$
$$\mathrm{J}_\pm^\dagger = \mathrm{J}_\mp \qquad !$$

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

$$\begin{aligned}\mathrm{J}_\mp\mathrm{J}_\pm &= \left(\mathrm{J}_x \mp i\mathrm{J}_y\right)\left(\mathrm{J}_x \pm i\mathrm{J}_y\right) = \mathrm{J}_x^2 + \mathrm{J}_y^2 \pm i\left[\mathrm{J}_x, \mathrm{J}_y\right] \\ &= \mathrm{J}^2 - \mathrm{J}_z^2 \pm i\left(i\hbar\mathrm{J}_z\right) = \mathrm{J}^2 - \mathrm{J}_z^2 \mp \hbar\mathrm{J}_z \\ &= \mathrm{J}^2 - \mathrm{J}_z\left(\mathrm{J}_z \pm \hbar\right)\end{aligned}$$

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

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

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

$e^{-i\delta_\pm}$: arbitrary phase factor that results 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:

known as the "Condon and Shortley" phase choice

(sometimes an alternative phase choice is used, $\delta_\pm = \pm\pi/2$, so be careful) standard phase choice: $\delta_{\pm} = 0$

$$\left\langle j'm' \middle| \mathbf{J}_{\pm} \middle| jm \right\rangle = \hbar \delta_{j'j} \delta_{m'm\pm1} \left[j(j+1) - m(m \pm 1) \right]^{1/2}$$

$$\left(\text{or } \hbar \delta_{jj'} \delta_{m'm\pm1} \left[j(j+1) - \underline{\underline{m(m')}} \right]^{1/2} \right)$$

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

Now, 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.

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

Summary

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

$$\left\langle jm \middle| \vec{\mathbf{J}} \middle| jm \right\rangle = \hat{k} \hbar m \qquad \left(\Delta m = 0 \text{ selects } \hat{k} \mathbf{J}_z \right)$$

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

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

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

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