Scalar Selection Rules

We had: $[\hat{L}_z, \hat{S}] = 0$ (1)

$[\hat{L}^2, \hat{S}] = 0$ (2)

$[\hat{L}_\pm, \hat{S}] = 0$ (3)

& putting these in: $\langle l'm' | \_\_ | lm \rangle$ gave:

$\hbar(m'-m)\langle l'm' | \hat{S} | lm\rangle = 0$ from (1)

$\hbar^2[l'(l'+1) - l(l+1)]\langle l'm' | \hat{S} | lm\rangle = 0$ from (2)

This pair tells us that $\langle l'm' | \hat{S} | lm\rangle = 0$ unless $m'=m$, $l'=l$.

For (3), we have:

$\langle l'm' | [\hat{L}_+, \hat{S}] | lm\rangle = 0$

"

$\underbrace{\langle l'm' | \hat{L}_+}_{= \langle \hat{L}_- l'm' | = B_{l'}^{m'} \langle l' m'-1 |} \hat{S} | lm\rangle - \langle l'm' | \hat{S} \underbrace{\hat{L}_+ | lm\rangle}_{= A_l^m | l\, m+1\rangle} = 0$

so

$B_{l'}^{m'} \underbrace{\langle l' m'-1 | \hat{S} | lm\rangle}_{=0 \text{ unless } m'-1=m,\ l'=l} - A_l^m \underbrace{\langle l'm' | \hat{S} | l\, m+1\rangle}_{=0 \text{ unless } m'=m+1,\ l'=l} = 0$

$B_l^{m+1} \langle lm | \hat{S} | lm\rangle - A_l^m \langle l\, m+1 | \hat{S} | l\, m+1\rangle = 0$

and $B_l^{m+1} = \hbar\sqrt{l(l+1) - (m+1)(m+1-1)} = A_l^m$

we learn that $\langle lm | \hat{S} | lm\rangle = \langle l\, m+1 | \hat{S} | l\, m+1\rangle$

Whatever $\langle lm | \hat{S} | lm\rangle$ is, it does not depend on m. Call the matrix elt.

$\langle lm | \hat{S} | lm\rangle \equiv \langle l \| \hat{S} \| l\rangle$

to highlight that independence. All together, we have:

$\langle l'm' | \hat{S} | lm\rangle = \delta_{ll'}\delta_{mm'} \langle l' \| \hat{S} \| l\rangle \ldots$

Example: the hydrogenic $|211\rangle$, $|210\rangle$, $|21-1\rangle$ are the 3 states w/ $n=2$, $l=1$

The selection rules tell us that

$\langle 21m' | \hat{S} | 21m\rangle = \delta_{mm'} \underbrace{\langle l=1 \| \hat{S} \| l=1\rangle}_{\text{same } \forall m}$

all we need to do is evaluate $\langle 1 \| \hat{S} \| 1\rangle$ for <u>one</u> m, & we're guaranteed it's the same $\forall m$.

Easiest is $m=0$ – take $\hat{S} = \hat{r}^2$, then

$\langle 210 | \hat{r}^2 | 210\rangle = \int_0^{2\pi}\int_0^{\pi}\int_0^{\infty} |\psi_{210}|^2 \cdot r^2 \sin\theta\, dr\, d\theta\, d\phi$

ends up being

$= 30 a^2 = \langle 1 \| \hat{r}^2 \| 1\rangle$

a is the Bohr radius.

& we know that

$\langle 210 | \hat{r}^2 | 210\rangle = \langle 211 | \hat{r}^2 | 211\rangle = \langle 21-1 | \hat{r}^2 | 21-1\rangle = 30a^2$

Clebsch-Gordon Recursion Relation

The definition of the C-G coefficients was:

$$|LM\rangle = \sum_{m_1,m_2} C^{l_1 l_2 L}_{m_1 m_2 M} \, |l_1 l_2 m_1 m_2\rangle \qquad (*)$$

the coefficients we need to make e-states of $\hat{L}^2 = (\vec{L}_1+\vec{L}_2)\cdot(\vec{L}_1+\vec{L}_2)$ & simultaneously, $\hat{L}_z = \hat{L}_{1z}+\hat{L}_{2z}$

We had $C^{l_1 l_2 L}_{m_1 m_2 M} = 0$ if $m_1+m_2 \neq M$

The states $|l_1 l_2 m_1 m_2\rangle$ are orthogonal, so

$$\langle l_1 l_2 m_1' m_2' | l_1 l_2 m_1 m_2\rangle = \delta_{m_1' m_1}\delta_{m_2' m_2}$$

& we can use this w/ $(*)$ to isolate the $C^{l_1 l_2 L}_{m_1 m_2 M}$:

$$\langle LM | l_1 l_2 m_1 m_2\rangle = C^{l_1 l_2 L}_{m_1 m_2 M}$$

Define: $\hat{L}_\pm = \hat{L}_{1\pm} + \hat{L}_{2\pm} = (\hat{L}_{1x} \pm i\hat{L}_{1y}) + (\hat{L}_{2x} \pm i\hat{L}_{2y})$

w/

$$\hat{L}_+|LM\rangle = A^M_L |L\, M+1\rangle \quad \text{w/ } A^M_L = \hbar\left(L(L+1)-M(M+1)\right)^{1/2}$$

$$\hat{L}_-|LM\rangle = B^M_\ell |L\, M-1\rangle \quad \text{w/ } B^M_L = \hbar\left(L(L+1)-M(M-1)\right)^{1/2}$$

then:

$$\hat{L}_+|LM\rangle = \sum_{m_1,m_2}(\hat{L}_{1+}+\hat{L}_{2+})\, C^{l_1 l_2 L}_{m_1 m_2 M} |l_1 l_2 m_1 m_2\rangle$$

$$A^M_L |L\, M+1\rangle = \sum_{m_1,m_2} C^{l_1 l_2 L}_{m_1 m_2 M}\left(A^{m_1}_{l_1}|l_1 l_2\, m_1+1\, m_2\rangle + A^{m_2}_{l_2}|l_1 l_2\, m_1\, m_2+1\rangle\right)$$

multiplying both sides by $\langle l_1 l_2 m_1' m_2'|$, we get

$$A^M_L \langle l_1 l_2 m_1' m_2' | L\, M+1\rangle = A^M_L C^{l_1 l_2 L}_{m_1' m_2' M+1}$$

$$+ \sum_{m_1,m_2} C^{l_1 l_2 L}_{m_1 m_2 M}\Big(A^{m_1}_{l_1}\underbrace{\langle l_1 l_2 m_1' m_2' | l_1 l_2\, m_1+1\, m_2\rangle}_{\delta_{m_1'\, m_1+1}\delta_{m_2' m_2}} + A^{m_2}_{l_2}\underbrace{\langle l_1 l_2 m_1' m_2' | l_1 l_2\, m_1\, m_2+1\rangle}_{\delta_{m_1' m_1}\delta_{m_2'\, m_2+1}}\Big)$$

$$= A^{m_1'-1}_{l_1} C^{l_1 l_2 L}_{m_1'-1\, m_2' M} + A^{m_2'-1}_{l_2} C^{l_1 l_2 L}_{m_1'\, m_2'-1\, M}$$

putting the 2 sides together gives:

$$A^M_L C^{l_1 l_2 L}_{m_1' m_2' M+1} = A^{m_1'-1}_{l_1} C^{l_1 l_2 L}_{m_1'-1\, m_2' M} + A^{m_2'-1}_{l_2} C^{l_1 l_2 L}_{m_1'\, m_2'-1\, M} \qquad (+)$$

&

$$A^{m'-1}_\ell = \hbar\left(\ell(\ell+1)-(m'-1)(m'-1+1)\right)^{1/2} = B^{m'}_\ell \quad \text{\& } (+) \text{ is}$$

$$A^M_L C^{l_1 l_2 L}_{m_1' m_2' M+1} = B^{m_1'}_{l_1} C^{l_1 l_2 L}_{m_1'-1\, m_2' M} + B^{m_2'}_{l_2} C^{l_1 l_2 L}_{m_1'\, m_2'-1\, M}.$$

Vector Selection Rules

For a vector operator $\hat{\vec{V}}$, w/ $\hat{V}_z$ & the linear combination

$$\hat{V}_\pm = \hat{V}_x \pm i\hat{V}_y$$

we have commutators (all stemming from $[\hat{L}_i, \hat{V}_j] = i\hbar\epsilon_{ijk}\hat{V}_k$

$$[\hat{L}_z, \hat{V}_z] = 0 \ , \quad [\hat{L}_z, \hat{V}_\pm] = \pm\hbar \hat{V}_\pm$$

$$[\hat{L}_\pm, \hat{V}_\pm] = 0 \quad [\hat{L}_\pm, \hat{V}_z] = \mp\hbar \hat{V}_\mp \quad [\hat{L}_\pm, \hat{V}_\mp] = 2\hbar \hat{V}_z$$

As before, we sandwhich these relations between $\langle l'm'|$ & $|lm\rangle$. The 1st one gives:

$$\langle l'm'| [\hat{L}_z, \hat{V}_z] |lm\rangle = 0$$

$$\parallel$$

$$\underbrace{\langle l'm'| \hat{L}_z}_{=\hbar m' \langle l'm'|} \hat{V}_z |lm\rangle - \langle l'm'| \hat{V}_z \underbrace{\hat{L}_z |lm\rangle}_{=\hbar m |lm\rangle} = 0$$

so $\hbar(m'-m) \langle l'm'| \hat{V}_z |lm\rangle = 0$

from which we learn that: $\langle l'm'| \hat{V}_z |lm\rangle = 0$ unless $m'=m$.

From the $[\hat{L}_z, \hat{V}_\pm] = \pm\hbar \hat{V}_\pm$, we get

$$\langle l'm'| [\hat{L}_z, \hat{V}_\pm] |lm\rangle = \pm\hbar \langle l'm'| \hat{V}_\pm |lm\rangle$$

$$\parallel$$

$$\underbrace{\langle l'm'| \hat{L}_z}_{=\hbar m' \langle l'm'|} \hat{V}_\pm |lm\rangle - \langle l'm'| \hat{V}_\pm \underbrace{\hat{L}_z |lm\rangle}_{=\hbar m |lm\rangle} = \pm\hbar \langle l'm'| \hat{V}_\pm |lm\rangle$$

$$\hbar(m'-m) \langle l'm'| \hat{V}_\pm |lm\rangle = \pm\hbar \langle l'm'| \hat{V}_\pm |lm\rangle$$

or $\hbar(m'-m \mp 1) \langle l'm'| \hat{V}_\pm |lm\rangle = 0$

which says: $\hbar(m'-(m+1)) \underbrace{\langle l'm'| \hat{V}_+ |lm\rangle}_{\substack{=0 \text{ unless} \\ m'=m+1}} = 0$

and: $\hbar(m'-(m-1)) \underbrace{\langle l'm'| \hat{V}_- |lm\rangle}_{=0 \text{ unless } m'=m-1} = 0$

using these & the recursion relations for the Clebsch-Gordon coeffs, we get:

$$\langle l'm'| \hat{V}_+ |lm\rangle = -\sqrt{2}\, C^{l1l'}_{m1m'} \langle l' \| \hat{V} \| l\rangle$$

$$\langle l'm'| \hat{V}_z |lm\rangle = C^{l1l'}_{m0m'} \langle l' \| \hat{V} \| l\rangle$$

$$\langle l'm'| \hat{V}_- |lm\rangle = \sqrt{2}\, C^{l1l'}_{m-1m'} \langle l' \| \hat{V} \| l\rangle$$

& keep in mind that $C^{l_1 l_2 L}_{m_1 m_2 M} = 0$ if $m_1 + m_2 \neq M$

and $C^{l_1 l_2 L}_{m_1 m_2 M} = 0$ if $L \neq l_1 + l_2 \ldots |l_1 - l_2|$

so the above are nonzero only if $\Delta m = 0, \pm 1$ & $\Delta l = 0, \pm 1$