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Quantum Mechanics 2

CH. 3 THE THEORY OF ANGULAR MOMENTUM LECTURE NOTES

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Angular Momentum States (Review)

Angular Momentum Operators, $\vec{J} = (J_x, J_y, J_z)$ are infinitesimal generators of rotations in the Hilbert space. If $R_{\hat{u}}(\theta)$ is the rotation operator in real space around a direction $\hat{u}$ by an angle θ, then

$$D(R) = \exp\left\{-\frac{i}{\hbar}\theta \vec{J}\cdot\hat{u}\right\}$$

describes a rotation in the Hilbert Space spanned by the eigenstates of one of the components of $\vec{J}$ (say J_z).

The J_i components $(i = x, y, z)$ satisfy

$$[J_i, J_j] = i\epsilon_{ijk} J_k$$

Where ϵ_{ijk} is the anti-symmetric tensor $\therefore$ J_x, J_y, J_z are incompatible operators and have different sets of eigenstates. On the other hand,

$$[J^2, J_i] = 0 \quad \text{where } J^2 = J_x^2 + J_y^2 + J_z^2$$

$\therefore$ J^2 and one of the components of $\vec{J}$ can be diagonalized simultaneously.

Choosing the basis of eigenstates of J_z, $|j,m\rangle$, the angular momentum operators satisfy the eigenvalue equation

$$J^2|j,m\rangle = \hbar^2 j(j+1)|j,m\rangle, \quad J_z|j,m\rangle = \hbar m|j,m\rangle$$

where j is the angular momentum quantum number and m is the magnetic quantum number.

In general, j is either a natural number: $j = 0, 1, 2, \ldots$ or a half integer: $j = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \ldots$

For a given value of j, there are $2j+1$ possible values of m: $-j \le m \le j$

<u>Definition</u>: Ladder Operators $J_\pm$

$$J_\pm = J_x \pm iJ_y$$

which satisfy: $[J_+, J_-] = 2\hbar J_z$, $[J_z, J_\pm] = \pm\hbar J_\pm$ and

$$J_\pm|j,m\rangle = \hbar\sqrt{(j\pm m+1)(j\mp m)}\,|j,m\pm1\rangle$$

The matrix elements of angular momentum operators are

$$\langle j',m'|J_\pm|j,m\rangle = \delta_{jj'}\delta_{m'm\pm1}\,\hbar\sqrt{(j\mp m)(j\pm m+1)}$$

$$\langle j',m'|J^2|j,m\rangle = \hbar^2 j(j+1)\delta_{jj'}\delta_{mm'} \ , \ \langle j',m'|J_z|j,m\rangle = \hbar m\,\delta_{mm'}\delta_{jj'}$$

<u>Example</u> ($j=1/2$) Spin 1/2

$$J_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \ , \ J^2 = \hbar^2 \frac{3}{4}\tilde{\mathbb{1}}$$

<u>Example</u> ($j=1$)

$$J_z = \hbar \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \ , \ J^2 = 2\hbar^2 \tilde{\mathbb{1}}$$

with magnetic quantum numbers $m = 0, \pm 1$.

<u>Addition of Angular Momentum</u> : Consider two different operators of angular momentum which operate in different Hilbert Spaces.

$$\vec{J} = \vec{J}_1 + \vec{J}_2 = \vec{J}_1 \otimes \vec{\mathbb{1}} + \mathbb{1} \otimes J_2$$

The components of $\vec{J}_1$ and $\vec{J}_2$ satisfy

$$[J_{1,i}, J_{1,j}] = \epsilon_{ijk} J_{1,k} \ , \ [J_{2,i}, J_{2,j}] = \epsilon_{ijk} J_{2,k}$$

with $i,j = x, y, z$. Since the operators act in different Hilbert spaces

$$[\vec{J}_1, \vec{J}_2] = 0$$

implying that

$$[J_i, J_j] = \epsilon_{ijk} J_k .$$

The total angular momentum is the infinitesimal generator of rotations in the extended Hilbert Space.

$$D(R) = D_1(R) \otimes D_2(R) = e^{-i/\hbar\, \sigma \vec{J}_1 \cdot \hat{u}} \otimes e^{-i/\hbar\, \sigma \vec{J}_2 \cdot \hat{u}} = \exp\left\{ \frac{-i}{\hbar} \sigma (\vec{J}_1 \otimes \tilde{\mathbb{1}} + \tilde{\mathbb{1}} \otimes \vec{J}_2) \cdot \hat{u} \right\} = \exp^{-i/\hbar\, \sigma \vec{J} \cdot \hat{u}}$$

<u>Total Angular Momentum Basis</u>

There are different representations for eigenstates in a system with two different angular momentum operators

i) choose a basis

$$|j_1, j_2; m_1, m_2\rangle \equiv |j_1, m_1\rangle \otimes |j_2, m_2\rangle$$

which diagonalizes a set of compatible operators:

$$\{ J_1^2, J_2^2, J_{1z}, J_{2z} \}$$

The eigenvalues of those operators are:

$$J_i^2 |j_1, j_2; m_1, m_2\rangle = \hbar^2 j_1(j_1+1) |j_1, j_2; m_1, m_2\rangle$$

$$J_{i,z} |j_1, j_2; m_1, m_2\rangle = \hbar m_1 |j_1, j_2; m_1, m_2\rangle$$

ii) Another option is to use the basis that diagonalizes a different set of compatible operators

$$\{J^2, J_z, J_1^2, J_2^2\}$$

Namely:

$$|j_1, j_2 : j, m\rangle$$

Where

$$J^2 |j_1, j_2; j, m\rangle = \hbar^2 j(j+1) |j_1, j_2; j, m\rangle$$

$$J_z |j_1, j_2; j, m\rangle = \hbar^2 j_1(j_1+1) |j_1, j_2; j, m\rangle$$

$$J_1^2 |j_1, j_2; j, m\rangle = \hbar^2 j_1(j_1+1) |j_1, j_2; j, m\rangle$$

$$J_2^2 |j_1, j_2; j, m\rangle = \hbar^2 j_2(j_2+1) |j_1, j_2; j, m\rangle$$

One can check that although

$$[J^2, J_z] = 0$$

the commutators

$$[J^2, J_{1z}] \neq 0, \quad [J^2, J_{2z}] \neq 0$$

Therefore the sets of operators to choices i) and ii) represent maximal sets of compatible operators. Hence, these should be a transformation that maps the two complete basis

$$|j_1, j_2; m_1, m_2\rangle \longleftrightarrow |j_1, j_2 : j, m\rangle$$

$$|j_1, j_2; j, m\rangle = \sum_{m_1, m_2} |j_1, j_2; m_1, m_2\rangle\langle j_1, j_2; m_1, m_2 | j_1, j_2; j, m\rangle$$

using the completeness relation of the basis.

<u>Definition</u>: Clebsh Gordan coefficients

$$\langle j_1, j_2; m_1, m_2 | j_1, j_2; j, m\rangle$$

<u>Properties of C.B. coefficients</u>

1.) The C.B. coefficients are zoo unless $m = m_1 + m_2$ since $J_z = J_{1z} + J_{2z}$

$0 = \langle j_1, j_2; m_1, m_2 | (J_z - J_{1z} - J_{2z}) | j_1, j_2; j, m\rangle = \langle j_1, j_2; m_1, m_2 | (\hbar m - \hbar m_1 - \hbar m_2) | j_1, j_2; j, m\rangle$

$= \hbar (m - m_1 - m_2) \langle j_1, j_2; m_1, m_2 | j_1, j_2; j, m\rangle$

Hence if $\langle j_1, j_2; m_1, m_2 | j_1, j_2; j, m\rangle \neq 0 \Rightarrow m = m_1 + m_2$

2.) The C.B coefficients are zero, except if

$$|j_1 - j_2| \leq j \leq j_1 + j_2$$

This statement implies the total number of states,

$$\sum_{|j_1 - j_2|, j_1 + j_2} 2j+1 = (2j_1+1)(2j_2+1)$$

One has $j_1 + j_2 - (j_1 - j_2) + 1 = 2j_2 + 1$ terms in the arithmatic series, with the average term

$$2\frac{(j_1 + j_2 + j_1 - j_2)}{2} + 1 = 2j_1 + 1$$

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__Clebsch__ __Gordon__ __coefficient__ __Properties__

3.) The C.G. coefficients form a unitary matrix.

By convention, the C.G. coefficients are real

$$\langle j_1, j_2; j, m | j_1, j_2; m_1, m_2\rangle = \langle j_1, j_2; m_1, m_2 | j_1, j_2; j, m\rangle$$

We have

$$\langle j_1, j_2; m_1, m_2 | j_1, j_2; m_1', m_2'\rangle = \delta_{m_1 m_1'} \delta_{m_2 m_2'}$$

$$= \sum_{j,m} \langle j_1, j_2; m_1, m_2 | j_1, j_2; j, m\rangle$$

Therefore the C.G coefficients are equal to them and orthogonal

$$\langle j_1, j_2; m_1, m_2 | j_1, j_2: j, m\rangle \equiv \langle m_1, m_2 | j, m\rangle$$

Hence

$$\sum_{j,m} \langle m_1, m_2 | j, m\rangle \langle m_1', m_2' | j, m\rangle = \delta_{m_1 m_1'} \delta_{m_2 m_2'}$$

__Recursion__ __Relations__ __For__ __C.G__ __Coefficients__

$$J_\pm |j, m\rangle = (J_{1\pm} + J_{2\pm}) \sum_{m_1 m_2} |m_1, m_2\rangle \langle m_1, m_2 | j, m\rangle$$

Since

$$J_\pm |j, m\rangle = \hbar \sqrt{(j \mp m)(j \pm m + 1)}\, |j, m \pm 1\rangle$$

$$\sqrt{(j\mp m)(j\pm m+1)}\,|j,m\pm1\rangle = \sum_{m_1,m_2}\sqrt{(j_1\mp m_1)(j_1\pm m_1+1)}\,|m_1\pm1,m_2\rangle + \sqrt{(j_2\mp m_2)(j_2\pm m_2+1)}\,|m_1,m_2\pm1\rangle \times \langle m_1,m_2|j,m\rangle$$

Multiplying the bra on the left then

$$\sqrt{(j\mp m)(j\pm m+1)}\,\langle m_1',m_2'|j,m\pm1\rangle = \sum_{m_1,m_2}\sqrt{(j_1\mp m_1)(j_1\pm m_1+1)}\times\langle m_1',m_2'|m_1\pm1,m_2\rangle\langle m_1,m_2|j,m\rangle$$

$$+\sum_{m_1,m_2}\sqrt{(j_2\mp m_2)(j_2\pm m_2+1)}\,\langle m_1',m_2'|m_1,m_2\pm1\rangle\times\langle m_1,m_2|j,m\rangle$$

Since,

$$\langle m_1',m_2'|m_1\pm1,m_2\rangle = \delta_{m_1',m_1\pm1}\,\delta_{m_2,m_2'}\ ,\quad \langle m_1',m_2'|m_1,m_2\pm1\rangle = \delta_{m_1'm_2}\,\delta_{m_2',m_2\pm1}$$

The C.G coefficients now become

$$\sqrt{(j\mp m)(j\pm m+1)}\,\langle m_1',m_2'|j,m\pm1\rangle = \sqrt{[j_1\mp(m_1'\mp1)][j_1\pm(m_1'\mp1)]}\,\langle m_1'\mp1,m_2'|j,m\rangle$$

$$+\sqrt{[j_2\mp(m_2'\mp1)][j_2\pm(m_2'\mp1)]}\,\langle m_1',m_2'\mp1|j,m\rangle$$

and hence :

$$\sqrt{(j\mp m)(j\pm m+1)}\,\langle m_1,m_2|j,m\pm1\rangle = \sqrt{(j_1\mp m_1+1)(j_1\pm m_1)}\,\langle m_1\mp1,m_2|j,m\rangle +$$

$$\sqrt{(j_2\mp m_2+1)(j_2\pm m_2)}\,\langle m_1,m_2\mp1|j,m\rangle$$

Which are the recursion relations to C.G coefficients where

$$m_1+m_2 = m\pm1$$

<u>Example</u> : $j_1=j_2=1/2$

The states are then

$$|j_1,j_2;J,M\rangle \equiv |J,M\rangle$$

A method (Ladder Operators)

$$J_\pm|J,M\rangle = \hbar\sqrt{(J\mp M)(J\pm M+1)}\,|J,M\pm1\rangle$$

Starting with the max M state with $M = 1/2 + 1/2 = 1$, then $J=1$

$$|1,1\rangle = |1/2,1/2;1/2,1/2\rangle$$

Now building the other $J=1$ kets

$$J_-|1,1\rangle = \hbar\sqrt{2}\,|1,0\rangle = (J_{1-}+J_{2-})|1/2,1/2\rangle$$

Applying J_- again,

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

This then implies that $|1,-1\rangle = |-\tfrac{1}{2},-\tfrac{1}{2}\rangle$

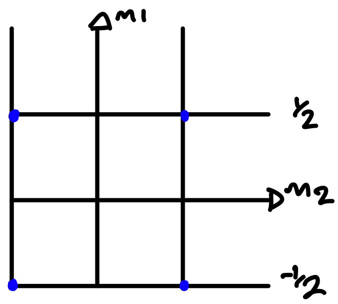
The Last state is $|0,0\rangle$ $(J=0)$ which is orthogonal to the $|1,0\rangle$ state

The 2nd Method

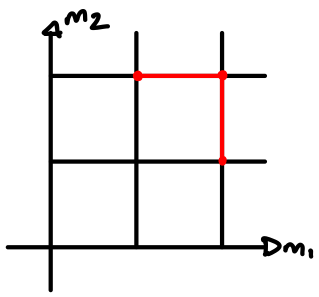
One can calculate C.G coefficients using expansion relations. Since $0 \le J \le 1 \Rightarrow J=0,1.$ Also, we have the selection rules,

$$|m_1| \le j_1,\ |m_2| \le j_2\ :\ -J \le M = m_1 + m_2 \le J$$

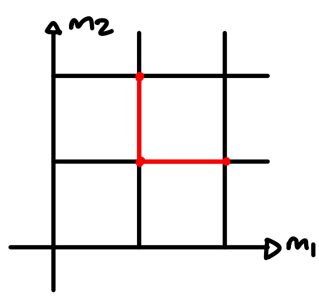
J=1



Solution Rules

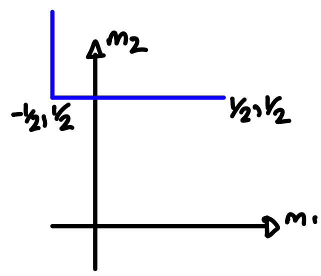


J_+



J_-

With $m_1 = \pm\tfrac{1}{2}$, $m_2 = \pm\tfrac{1}{2}$ $(J=1)$



For $(m_1, m_2) = (-\tfrac{1}{2}, \tfrac{1}{2})$, $m_1 + m_2 = m - 1 = 0$ (J_-) $\Rightarrow m = 1$

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Tensor Operators

Vector Operators: A regular vector that transforms as

$$V_i \rightarrow \sum_j R_{ij} V_j = V_i$$

Where R_{ij} is an orthogonal matrix associated with the rotation.

The rotation of a ket $|\alpha\rangle$ is

$$|\alpha\rangle \rightarrow |\alpha'\rangle = D(R)|\alpha\rangle \Rightarrow \langle\alpha'|V_i|\alpha'\rangle = \langle\alpha|D^\dagger(R)V_i D(R)|\alpha\rangle$$

For a vector operator,

$$\langle\alpha|D^\dagger(R)V_i D(R)|\alpha\rangle = \sum_j R_{ij}\langle\alpha|V_j|\alpha\rangle$$

For all kets $|\alpha\rangle$

$$D^\dagger(R)V_i D(R) = \sum_j R_{ij}V_j.$$

Considering an infinitesimal rotation

$$D(R) = \tilde{\mathbb{1}} - \underset{K}{\frac{i}{}}\, H(\underset{J_m}{\vec{J}\cdot\hat{m}})$$

and expanding to first order in H,

$$D^\dagger(R)V_i D(R) = (1+\frac{i}{\hbar}HJ_m)V_i(1-\frac{i}{\hbar}HJ_m) = V_i + \frac{H}{i\hbar}[V_i, J_m] + \mathcal{O}(H^2) = \sum_i R_{ij}(H,\hat{m})V_j$$

For a rotation around $\hat{z}$,

$$R_{ij} = \begin{pmatrix} \cos(\theta) & -\sin(\theta) & 0 \\ \sin(\theta) & \cos(\theta) & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad H \rightarrow 0 \longrightarrow \begin{pmatrix} 1 & -H & 0 \\ H & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \sum_j R_{ij}V_j \rightarrow \begin{pmatrix} V_x - HV_y \\ V_y + HV_x \\ V_z \end{pmatrix}$$

we get:

$$V_x + \frac{H}{i\hbar}[V_x, J_z] = V_x - HV_y, \quad V_y + \frac{H}{i\hbar}[V_y, J_z] = V_y + HV_x, \quad V_z + \frac{H}{i\hbar}[V_z, J_z] = V_z$$

This then implies

$$[V_x, J_z] = -i\hbar V_y, \quad [V_y, J_z] = i\hbar V_x, \quad [V_z, J_z] = 0$$

For an arbitrary direction we can say,

$$[V_i, J_j] = i\hbar\epsilon_{ijk}V_k$$

For any vector operator.

<u>Cartesian Tensors</u>: A given tensor of order M, $T_{ijk\ldots}$ transforms as:

$$T_{ijk\ldots} \longrightarrow \sum_{i'j'k'} R_{ii'}R_{jj'}R_{kk'} \times T_{i'j'k'\ldots}$$

Where R_{ij} is an orthogonal matrix.

<u>Example: Diadic Product of Two Vectors</u>

$$T_{ij} = V_i V_j = (\overset{\leftrightarrow}{u}\cdot V)_{ij}$$

Cartesian tensors are reducible under rotations, and hence can be broken into terms that transform differently under rotations. A vector operator V_i it transforms under an irreducible representation of dimension 3.

Since

$$D^\dagger(R) V_i D(R) = \sum_j R_{ij} V_j$$

then the generator of rotations whose rotation operator $D(R)$ has an irreducible representation of dimension 3, corresponds to an angular momentum operator with $j=1$.

Since

$$u_i = \sum_{i} R_{ii'} u_{i'} = D^{\dagger(1)} u_i D^{(1)} \Rightarrow u_i V_j = \sum_{ii'} \sum_{jj'} R_{ii'} R_{jj'} u_{i'} V_{j'} = [D^{(1)} \otimes D^{(1)}]^\dagger (u_i V_j) [D^{(1)} \otimes D^{(1)}]$$

Therefore, in the operator space $u_i V_j$ is a basis for the product space of two angular momentum operators with $j_1 = 1$ and $j_2 = 1$

$$\vec{J} = \vec{J}_1 + \vec{J}_2$$

Where $j = 0, 1, 2$, and $|j_1 - j_2| \leq j \leq j_1 + j_2$.

The product space spamed by the diadic $V_i V_j$ can be broken into three irreducible representations with dimensions 1, 2, 3

$$\Rightarrow D^{(1)}(R) \otimes D^{(1)}(R) = D^{(0)}_{(R)} \oplus D^{(1)}_{(R)} \oplus D^{(2)}_{(R)}.$$

In general,

$$D^{(j_1)} \otimes D^{(j_2)} \rightarrow \sum_{j=|j_1 - j_2|}^{j_1 + j_2} D^{(j)}$$

Indeed,

$$V_i V_j = \frac{\vec{u}\cdot\vec{v}}{3}\delta_{ij} + \frac{u_i V_j - u_j V_i}{2} + \frac{u_i V_j + u_j V_i}{2} - \frac{\vec{u}\cdot\vec{v}}{3}\delta_{ij}$$

we have:

i) $j=0$: invariant under rotation $T^{(0)} = \vec{u}\cdot\vec{v} = \sum_{i=1,2,3} u_i V_i$

ii) $j=1$: anti-symmetric tensors which transform like vectors,

$$T^{(1)}_{ij} = \frac{1}{2}(u_i V_j - u_j V_i) \rightarrow \vec{u} \times \vec{v}$$

three independent components.

iii) $j=2$: Symmetric tensors (traceless)

$$T_{ij}^{(2)} = \frac{1}{2}(u_i v_j + u_j v_i) - \frac{\vec{u}\cdot\vec{v}}{3}\delta_{ij}$$

$\rightarrow$ 5 independent components. $T^{(j)}$ is a spherical tensor of order j.

<u>Building Spherical Tensors From Spherical Harmonics</u>

<u>Def</u>: Wegman rotation

$$D(R)\psi(\vec{n}) \equiv \langle \vec{n} | D(R) | \psi \rangle \quad \text{w/} \quad D(R)|\vec{n}\rangle = |R\vec{n}\rangle$$

$$\Rightarrow \langle \vec{n} | D(R) = (D^{+}(R)|\vec{n}\rangle)^{+} = (D^{-1}(R)|\vec{n}\rangle)^{+} = \langle R^{-1}\vec{n}|$$

$$D(R)\psi(\vec{n}) = \langle R^{-1}\vec{n}|\psi\rangle = \psi(R^{-1}\vec{n})$$

Spherical Harmonics Rotate Like:

$$D(R) X_m^{\ell}(\hat{u}) = \langle \hat{u} | D(R) | \ell, m \rangle = \sum_{-\ell < m' < \ell} \langle \hat{u} | \ell, m' \rangle \langle \ell, m' | D(R) | \ell, m \rangle = \sum_{-\ell < m' < \ell} Y_{m'}^{\ell}(\hat{u}) D_{m m'}^{(\ell)}(R)$$

$$Y_m^{\ell}(R^{-1}\hat{u}) = \sum_{-\ell < m' < \ell} Y_{m'}^{\ell}(\hat{u}) D_{m' m}^{\ell}(R)$$

which is the same way spherical tensors rotate.

One can build spherical tensors of order ℓ by unitary spherical Harmonics $Y_m^{\ell}(\hat{u})$ with the unit vector $\hat{u}$ replaced by a vector operator $\vec{V}$,

$$T_m^{(\ell)} = Y_m^{(\ell)}(\vec{V})$$

where $\vec{V}$ is a vector operator.

<u>Example</u> : $\ell = 1$

In Spherical co-ordinates

$$u_x = \sin(\theta)\cos(\varphi), \quad u_y = \sin(\theta)\sin(\varphi), \quad u_z = \cos(\theta)$$

$$Y_{\pm 1}^{0}(\theta,\varphi) = \sqrt{\frac{3}{4\pi}}\cos(\theta) = \sqrt{\frac{3}{4\pi}}\,u_z, \quad Y_0^{\pm 1}(\theta,\varphi) = \mp\sqrt{\frac{3}{8\pi}}e^{i\varphi}\sin(\theta) = \sqrt{\frac{3}{8\pi}}(u_x + u_y)$$

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In general, the generalized rotation of spherical tensor operators is:

$$D(R) Y_\ell^{m}(\vec{v}) D^{+}(R) = \sum_{m'} Y_\ell^{m'}(\vec{v}) D_{m' m}^{(\ell)}(R)$$

<u>Definition:</u> Spherical tensors of order K : $T_q^{(K)}$ are objects that transform like:

$$D(R)T_q^{(k)}D^\dagger(R) = \sum_{-k<q<k} T_q^{(k)} D_{q'q}^{(k)}(R)$$

where

$$D_{qq'}^{(k)} \equiv \langle kq | D(R) | kq' \rangle$$

Using infinitesimal rotations,

$$(\mathbb{1} - \frac{i}{\hbar}\delta\varphi J_u) T_q^{(k)} (\mathbb{1} + \frac{i}{\hbar}\delta\varphi J_u) = \sum_{q'} T_{q'}^{(k)} \langle kq' | D(\delta\varphi \hat{u}) | kq \rangle$$

$$= \sum_{q'} T_{q'}^{(k)} \langle kq' | (1 - \frac{i\delta\varphi J_u}{\hbar}) | kq \rangle = T_q^{(k)} - \frac{i\delta\varphi}{\hbar} \sum_i T_{q'}^{(k)} \langle kq' | J_u | kq \rangle$$

$$= T_q^{(k)} - \frac{i}{\hbar}\delta\varphi [J_u, T_q^{(k)}] \Rightarrow [J_u, T_q^{(k)}] = \sum_{q'} \langle kq' | J_u | kq \rangle \times T_{q'}^{(k)}$$

$$\text{Fa } \hat{u} \Rightarrow J_z |kq\rangle = \hbar q |kq\rangle$$

Finally we have,

$$[T_q^{(k)}, J_z] = -\hbar q T_q^{(k)} \qquad (1)$$

W/ Fa $\hat{u} = x \pm y \Rightarrow J_{\hat{u}} = J_\pm$

$J_\pm |kq\rangle = \hbar \sqrt{(k \mp q)(k \pm q + 1)} \, |k, q \pm 1\rangle$, $\langle kq' | J_\pm | kq \rangle = \hbar \sqrt{(k \mp q)(k \pm q + 1)} \, \delta_{q', q \pm 1}$

This turns into finally,

$$[T_q^{(k)}, J_\pm] = -\hbar \sqrt{(k \mp q)(k \pm q + 1)} \, T_{q \pm 1}^{(k)} \qquad (2)$$

Which are alternative definitions of spherical tensors.

Products of Spherical Tensors

In general, products of spherical tensors

$$T_{q_1}^{(k_1)} Z_{q_2}^{(k_2)} \longleftrightarrow ?$$

are reducible tensors.

Theorem: Two irreducible spherical tensors $X_{q_1}^{(k)}$ and $Z_{q_2}^{(k)}$ of order k_1 and k_2, then

$$T_q^{(k)} = \sum_{q_1, q_2} X_{q_1}^{(k_1)} Z_{q_2}^{(k_2)} \times \langle k_1, k_2 ; q_1, q_2 | k_1, k_2 ; kq \rangle$$

is a spherical tensor of order k.

The C.G coefficients satisfy the selection rules:

i) k such that : $|k_1 - k_2| \leq k \leq k_1 + k_2$

ii) $q = q_1 + q_2$

Proof: Since,

$$|k_1,k_2;kq\rangle = \sum_{q_1q_2} \underbrace{|k_1,k_2;q_1,q_2\rangle}_{\to\, |k_1,q_1\rangle\otimes|k_2,q_2\rangle}\langle k_1,k_2;q_1,q_2|$$

then multiplying by $\langle\hat{m}|$,

$$Y_k^q(\hat{m}) = \sum_{q_1q_2} Y_{q_1}^{k_1} Y_{q_2}^{k_2} \langle\ldots\rangle$$

The same relation is valid for spherical tensor products.

Matrix Elements For Spherical Tensors

In many problems, we need to compute matrix elements of tensor operators among states of angular momenta. There are a few selection rules.

(I) m selection Rule:

$$\langle\alpha';j'm'|T_q^{(k)}|\alpha,jm\rangle = 0$$

unless $m' = m+q$

Proof Since

$$[T_q^{(k)},J_z] + \hbar q T_q^{(k)} = 0$$

$$0 = \langle\alpha',j'm'|([T_q^{(k)},J_z]+\hbar q T_q^{(k)})|\alpha,jm\rangle = \hbar(m-m'+q)\times\langle\alpha',j'm'|T_q^{(k)}|\alpha,jm\rangle$$

$$\text{If } m'\neq m+q \Rightarrow \langle\alpha',j'm'|T_q^{(k)}|\alpha,jm\rangle = 0$$

Wigner Eckhart Theorem

If $T_q^{(k)}$ is an irreducible spherical tensor of order k. It's matrix elements with respect to angular momentum states satisfy:

$$\langle\alpha',j'm'|T_q^{(k)}|\alpha,jm\rangle = \langle jk,mq|jk,j'm'\rangle\times\frac{\langle\alpha'j'\|T^{(k)}\|\alpha j\rangle}{\sqrt{2j+1}}$$

where $\langle jk,mq|jk,j'm'\rangle$ is the CG coefficient of addition of angular momenta

$$D^{(j)}\otimes D^{(k)} = \sum_{j'=|j-k|}^{j+k} D^{(j')}$$

$\Rightarrow$ Selection rule for j'. This term is purely geometric and depends on angular momenta projections along a given direction

The second term $\langle\alpha'j'\|T^{(k)}\|\alpha j\rangle$ depends on the dynamics of the system through quantum number α, but not on magnetic quantum numbers (m,m',q).

Proof:

$$\langle \alpha', j'm' | [J_\pm, T_q^{(k)}] | \alpha, jm \rangle = \hbar\sqrt{(k\mp q)(k\pm q+1)}\, \langle \alpha', j'm' | T_{q\pm1}^{(k)} | \alpha', jm \rangle$$

$$= \hbar\sqrt{(j'\pm m')(j'\mp m'+1)}\, \langle \alpha', j'm'\mp1 | T_q^{(k)} | \alpha', jm \rangle - \hbar\sqrt{(j'\mp m')(j'\pm m'+1)}\, \langle \alpha', j'm' | T_q^{(k)} | \alpha, jm \rangle$$

Exchanging $+ \leftrightarrow -$,

$$\sqrt{(j'\mp m')(j'\pm m'+1)}\, \langle \alpha', j'm'\pm1 | T_q^{(k)} | \alpha, jm \rangle =$$

$$\sqrt{(k\pm q)(k\mp q+1)}\, \langle \alpha', j'm' | T_{q\pm1}^{(k)} | \alpha, jm \rangle + \sqrt{(j\pm m)(j\mp m+1)}\, \langle \alpha', j'm' | T_q^{(k)} | \alpha, jm\mp1 \rangle$$

This expression has the same form as the recursion relation for C. G. coefficients by exchanging

$j \to j'$ $\qquad (j_1, j_2) \to (j, k)$, $(m_1, m_2) \to (m, q)$ $\qquad m \to m'$

$$\sqrt{(j'\mp m')(j'\pm m'+1)} \times \langle jk; mq | jk, j'm'\pm1 \rangle =$$

$$\sqrt{(k\pm q)(k\mp q+1)} \times \langle jk, m, q\pm1 | jk, j'm' \rangle + \sqrt{(j\pm m)(j\mp m+1)}\, \langle jk, m\pm1, q | jk, j'm' \rangle$$

The two first order homogeneous equations, have the form

$$\sum_{j=1}^{3} a_{ij} x_j = 0 \,,\ \sum_{j=1}^{3} a_{ij} y_j = 0$$

Solving for the ratios,

$$\frac{x_j}{x_k} \text{ and } \frac{y_j}{y_k}$$

The solutions must be unique $\frac{y_j}{y_k} = \frac{x_j}{x_k} \Rightarrow y_j = \left(\frac{y_k}{x_k}\right) x_j = c_k x_j$ where c is a constant.

$$\langle \alpha', j', m'\pm1 | T_q^{(k)} | \alpha, j, m \rangle = C_{\alpha\alpha'}(jk, j') \times \langle jk, mq | jk, j'm'\pm1 \rangle$$

Where by convention:

$$C_{\alpha\alpha'}(jk, j') \equiv \frac{\langle \alpha' j' \| T^{(k)} \| \alpha, j \rangle}{\sqrt{2j+1}}$$

Example: (spinless particle)

$$\langle n' l' m' | T_q^{(l)} | n l m \rangle = \langle l, mq | l, l'm' \rangle \times \frac{\langle n' l' \| T^{(1)} \| n l \rangle}{\sqrt{2l+1}}$$

Selection rules $\langle l_1, mq | l_1, l'm' \rangle = 0$ unless:

a) $m' = m + q$

b) $l' = |l \pm 1|, l$

Parity Selection Rule: The parity operator is related to spatial inversion

$$(x,y,z) \Rightarrow (-x,-y,-z)$$

It is Hermitian and Idempotent, i.e.

$$P^2 = \mathbb{I}.$$

Any vector operator is odd under parity,

$$P T_q^{(1)} P = - T_q^{(1)}.$$

As spherical harmonics,

$$P|l,m\rangle = (-1)^l |l,m\rangle$$

Hence

$$\langle \alpha' l' m' | P T_q^{(1)} P | \alpha l m\rangle = - \langle \alpha' l' m' | T_q^{(1)} | \alpha l m\rangle = (-1)^l (-1)^{l'} \langle \alpha' l' m' | T_q^{(1)} | \alpha l m\rangle$$

$$= (-1)^{l+l'} \langle \alpha' l' m' | T_q^{(1)} | \alpha l m\rangle$$

$\Rightarrow$ The matrix elements are zero unless $l + l' = 2n+1$, $n \in \mathbb{Z}$

In that case the selection rule discards the case $l' = l$, $l' = |l \pm 1|$, $m' = m + q$