Angular Momentum

Let's now return to angular momentum. Much of what we do in this chapter is review, although we may approach the material from a slightly different direction. We defined the angular momentum operators as:

i) being the generators of rotations
ii) hence having a set of commutation relations

$$[\hat{J}_\alpha, \hat{J}_\beta] = i\epsilon_{\alpha\beta\gamma}\hat{J}_\gamma .$$

The operator $\hat{J}^2 = \hat{J}_x^2 + \hat{J}_y^2 + \hat{J}_z^2$ commutes with all $\hat{J}_\alpha$ and hence they have a common set of eigenvectors. But because of the commutation relations, there are only 2 sets of eigenvalues. We choose

$$\hat{\vec{J}}^2 |\beta, m\rangle = \beta\hbar^2 |\beta, m\rangle$$
$$\hat{J}_z |\beta, m\rangle = m\hbar |\beta, m\rangle .$$

Now, since

$$\beta\hbar^2 = \langle\beta, m|\hat{\vec{J}}^2|\beta, m\rangle = \sum_\alpha \langle\beta, m|\hat{J}_\alpha^2|\beta, m\rangle$$
$$= m^2\hbar^2 \langle\beta, m|\beta, m\rangle + \sum_{x,y} \underline{\langle\beta, m|\hat{J}_\alpha^2|\beta, m\rangle}$$

This is positive,
$\langle\beta, m|\hat{J}_\alpha^2|\beta m\rangle = (\langle\beta m|\hat{J}_\alpha^\dagger)(\hat{J}_\alpha|\beta m\rangle) \geq 0$.

$$\Rightarrow \quad \beta \geq 0$$
$$\beta \geq m^2 .$$

Proceeding as we did with the harmonic oscillator problem, (similarly to, anyway) we define

$$\hat{J}_+ = \hat{J}_x + i\hat{J}_y$$
$$\hat{J}_- = \hat{J}_x - i\hat{J}_y$$

which satisfy:

$$[\hat{J}_z, \hat{J}_+] = [\hat{J}_z, \hat{J}_x] + i[\hat{J}_z, \hat{J}_y] = i\hbar[\hat{J}_y + i(-J_x)]$$
$$= \hbar(J_x + iJ_y) = \hbar\hat{J}_+$$

$$[\hat{J}_z, \hat{J}_-] = -\hbar\hat{J}_-$$

$$[\hat{J}_+, \hat{J}_-] = [\hat{J}_x, \hat{J}_x] + i[\hat{J}_y, \hat{J}_x] - i[\hat{J}_x, \hat{J}_y] + [\hat{J}_y, \hat{J}_y]$$
$$= 0 + i(-i\hbar\hat{J}_z) - i(i\hbar\hat{J}_z) + 0$$
$$= 2\hbar\hat{J}_z.$$

Now, the effect of $\hat{J}_+$ is to change the value of m:

$$\hat{J}_z(\hat{J}_+|\beta, m\rangle) = \hat{J}_+\hat{J}_z|\beta, m\rangle + \hbar\hat{J}_+|\beta, m\rangle$$
$$= \hat{J}_+(m\hbar + \hbar)|\beta, m\rangle = (m+1)\hbar\hat{J}_+|\beta, m\rangle$$

Now, for a given β there is a maximum value of m ($\beta \geq m^2$). Hence, at some ~~point~~ value of m we must have

$$J_+|\beta, m\rangle = 0$$

Call that value of $m = j$. To find the relation between β and j, use

$$\hat{J}_-\hat{J}_+ = \hat{J}_x^2 + i\hat{J}_x\hat{J}_y - i\hat{J}_y\hat{J}_x + \hat{J}_y^2$$
$$= (\hat{J}_x^2 + \hat{J}_y^2) + i[\hat{J}_x, \hat{J}_y]$$
$$= \hat{J}^2 - \hat{J}_z^2 + i(i\hbar\hat{J}_z)$$
$$= \hat{\vec{J}}^2 - \hat{J}_z^2 - \hbar\hat{J}_z.$$

Apply $\hat{J}_-\hat{J}_+$ to $|\beta, j\rangle$ gives $\nearrow 0 \quad (J_+|\beta, j\rangle = 0)$

$\searrow \beta\hbar^2 - j^2\hbar^2 - \hbar(j\hbar)$

$$\Rightarrow \quad \beta = j(j+1)$$

By similar reasoning, we can show that

$$\hat{J}_- |\beta, -j\rangle = 0$$

But since $\hat{J}_+$ and $\hat{J}_-$ change m by an integer, then the set of eigenvalues for m must be

m	m	m	m
			$+3/2$
	$+1/2$	$+1$	$+1/2$
0	$-1/2$	0	$-1/2$
		-1	$-3/2$

etc.

$\Rightarrow \quad j = 0 \qquad j = 1/2 \qquad j = 1 \qquad j = 3/2$

Let's now call $|j, m\rangle$ our set of eigenvectors instead of $|\beta, m\rangle$. Note that we have obtained all of this without reference to spherical harmonics or other specific representations of $|j, m\rangle$.

Lastly, we can find the explicit action of $\hat{J}_+ |j, m\rangle$ by using $\langle j, m | \hat{J}_+^{\dagger} \hat{J}_+ | j, m\rangle \quad (\hat{J}_+ = \hat{J}_-^{\dagger})$.

$$= \langle j, m-1 | C_+^* \cdot C_+ | j, m-1\rangle = |C_+|^2 .$$

But $\hat{J}_- \hat{J}_+ = \hat{\vec{J}}^2 - \hat{J}_z^2 - \hbar \hat{J}_z$

$$\Rightarrow \quad C_\pm = \hbar \left[j(j+1) - m(m \pm 1) \right]^{1/2} \qquad \left(\begin{array}{l}\text{choosing the} \\ \text{phase of } C \\ \text{to be real}\end{array}\right).$$

Orbital and Spin Angular Momentum

Back in the discussion of commutators, we could have derived (but we didn't; see Ballentine for proof):

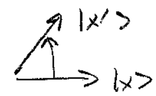
$$\hat{\vec{J}} = \vec{L} = \hat{\vec{Q}} \times \hat{\vec{P}}$$

for particles with no spin structure. Let's examine how the ang. mom. $\vec{J}$ changes states etc. The rotation transformation was defined by

$$\hat{R}_{\vec{u}}(\theta) = e^{-i\theta \hat{\vec{J}}\cdot\vec{u}/\hbar}$$

where $\vec{u}$ is the unit vector along the axis of rotation. Now, if we operate

$$\hat{R}\,|\vec{x}\rangle \rightarrow |\vec{x}\,'\rangle$$



or, operating on a single component wavefunction

$$\hat{R}\,\psi(\vec{x}) = \psi'(\vec{x}) = \psi(\hat{R}^{-1}\vec{x}) \quad \left(\text{for the usual reasons}\right).$$

Aside: Say we rotate around the z-axis by an angle $+\epsilon$

$$R_z\psi(\vec{x}) = \psi(x\cos\epsilon + y\sin\epsilon\,,\ -x\sin\epsilon + y\cos\epsilon\,,\ z)$$

$$\xrightarrow[\epsilon\to 0]{} \psi(x+\epsilon y\,,\ -\epsilon x + y\,,\ z)$$

$$= \psi(x,y,z) + \epsilon y\frac{\partial\psi}{\partial x} - \epsilon x\frac{\partial\psi}{\partial y}$$

$$= \psi(x,y,z) + i\epsilon\underbrace{\left[y\left(-i\frac{\partial}{\partial x}\right) - x\left(-i\frac{\partial}{\partial y}\right)\right]}_{\rightarrow\, i\hbar\epsilon\,(y\hat{p}_x - x p_y)\ \rightarrow\ -i\hbar\epsilon\hat{J}_z}\psi$$

as expected in this representation

For a multicomponent wavefunction, we can have

$$\psi = \begin{pmatrix} \psi_1(\vec{x}) \\ \psi_2(\vec{x}) \\ \vdots \end{pmatrix}$$

$$\hat{R}\psi = \hat{R}\begin{pmatrix} \psi_1(\vec{x}) \\ \psi_2(\vec{x}) \end{pmatrix} = \hat{D}\begin{pmatrix} \psi_1(R^{-1}\vec{x}) \\ \psi_2(R^{-1}\vec{x}) \\ \vdots \end{pmatrix}$$

This matrix $\hat{D}$ mixes up different components of the wavefunction.
If we demand that $\hat{D}$ be ~~Hermitian~~ unitary, then we write it in the form

$$D_u(\theta) = e^{-i\theta\vec{S}\cdot\vec{u}/\hbar}$$

must be Hermitian with 3 components S_x, S_y, S_z; each S_α may be $n \times n$.

Combining R and D, the general form of $\vec{J}$ is

$$\vec{J} = \vec{L} + \vec{S}$$

spin angular momentum: intrinsic to system

usual $\hat{\vec{Q}} \times \hat{\vec{P}}$, orbital angular momentum with respect to some origin

This is the part of $\vec{J}$ operating on the coordinates $\vec{x}$.

$\vec{L}$ and $\vec{S}$ commute.

What are the eigenvalues for these operators $\hat{L}$ and $\hat{S}$?
In the wavefunction approach, restrictions on $\hat{L}$ are obtained by demanding that the $Y_{\ell m}$'s of the angular differential equation be:

single valued $\rightarrow$ m is an integer
non-singular $\rightarrow$ $\ell \geq |m|$.

But, in our approach it is only $\langle \psi | \hat{A} | \psi \rangle$ which counts, and this quantity is unchanged even if ψ does change by a sign under rotation by $\varphi = 2\pi$. In other words, $Y_{1/2,1/2}$ ($\ell = 1/2$, $m = 1/2$) $= (\sin\theta)^{1/2} \exp(i\varphi/2)$ forms perfectly acceptable values of $\langle \psi | A | \psi \rangle$. How do we exclude it?

To find the extra restriction, we use
i) commutation relations for $\hat{I}_\alpha$
+ ii) $\hat{L} = \hat{Q} \times \hat{P}$ and their commutation relations.

Suppose we look at $\hat{L}_z = \hat{Q}_x \hat{P}_y - \hat{Q}_y \hat{P}_x$

If we adopt (where Q and P are rescaled by factors of m and c to make them have the same units of $\sqrt{\hbar}$.)

$$q_1 = \frac{Q_x + P_y}{\sqrt{2\hbar}} \qquad Q_x = \sqrt{\frac{\hbar}{2}}(q_1 + q_2)$$

$$q_2 = \frac{Q_x - P_y}{\sqrt{2\hbar}} \qquad P_y = \sqrt{\frac{\hbar}{2}}(q_1 - q_2)$$

q & p are dimensionless.

$$p_1 = \frac{P_x - Q_y}{\sqrt{2\hbar}} \qquad P_x = \sqrt{\frac{\hbar}{2}}(p_1 + p_2)$$

$$p_2 = \frac{P_x + Q_y}{\sqrt{2\hbar}} \qquad Q_y = -\sqrt{\frac{\hbar}{2}}(p_1 - p_2)$$

In Harm Osc. $\hat{p} \rightarrow \left(\frac{1}{M\hbar\omega}\right)^{1/2}\hat{P}$, $\hat{q} \rightarrow \left(\frac{M\omega}{\hbar}\right)^{1/2}\hat{Q}$

$$\hat{L}_z = \frac{\hbar}{2}\left(q_1^2 - q_2^2 + (-1)^2[p_1^2 - p_2^2]\right) = \frac{\hbar}{2}\left([p_1^2 + q_1^2] - [p_2^2 + q_2^2]\right)$$

where we have used $[q_\alpha, q_\beta] = [p_\alpha, p_\beta] = 0$.

The form of this operator is the same as that of the 1-D harmonic oscillator. So do same replacement with creation and destruction operators (pg. 6-1) to find

$$\hat{q}_1^2 + \hat{p}_1^2 = n_1 + 1/2 \qquad q_2^2 + p_2^2 = n_2 + 1/2 \qquad n_1, n_2 = 0, 1, 2 \cdots$$

$$\Rightarrow \quad L_z = (n_1 - n_2)\hbar \qquad n_1, n_2 = 0, 1, 2, 3 \cdots$$

This implies that L_z must come in integer multiples of $\hbar$, (rules out $L_z = 1/2$ etc.).

Spin Angular Momentum $\vec{S}$

$\vec{S}$ has been introduced just as $\vec{J}$ has, so we expect

$$\hat{\vec{S}}^2 |s, m_s\rangle = \hbar^2 s(s+1) |s, m_s\rangle \qquad m_s = s, s-1 \cdots -s.$$
$$\hat{S}_z |s, m_s\rangle = \hbar m_s |s, m_s\rangle.$$

Now, the additional constraint imposed by $L = Q \times P$ is missing, so $s = 1/2, 1, 3/2 \cdots$
The spin operators $\vec{S}$ operates on a $2s+1$ - dimensional space spanned by $|s, m_s\rangle$. However, there are only 3 $\vec{S}$'s for any $2s+1$ set of eigenvectors. Some examples:

$S = 1/2$

A representation of $\vec{S}$ is $\vec{S} = \frac{1}{2}\hbar\vec{\sigma}$

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

The spin eigenvectors can be shown to have the form (Ballentine, pg. 128-9)

$$\begin{pmatrix} e^{-i\varphi/2} \cos\frac{\theta}{2} \\ e^{i\varphi/2} \sin\frac{\theta}{2} \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} -e^{-i\varphi/2} \sin\frac{\theta}{2} \\ e^{i\varphi/2} \cos\frac{\theta}{2} \end{pmatrix}.$$

Note that there is a one-to-one correspondence between φ, θ to specify the eigenvector, and φ, θ to specify a 2-D vector of unit length. For a 2D vector, see (A) on pg (7-8A)

The density matrix ρ corresponding to 2 states is

$$\rho = \frac{1}{2}\Big(\underbrace{\mathbb{1}}_{2\times 2} + \underbrace{\vec{\pi}}_{\text{scalar}} \cdot \underbrace{\vec{\sigma}}_{2\times 2}\Big).$$

What is the significance of π? $\langle S_\alpha \rangle$

$$= \frac{\hbar}{2} \cdot \mathrm{Tr}(\rho S_\alpha)$$

$$= \frac{\hbar}{4} \mathrm{Tr}\left(\mathbb{1}\sigma_\alpha + \pi_x \sigma_x \sigma_\alpha + \pi_y \sigma_y \sigma_\alpha + \pi_z \sigma_z \sigma_\alpha \right)$$

These are each proportional to σ, except where $\sigma_\alpha \cdot \sigma_i \Rightarrow \mathbb{1}$. Others have $\mathrm{Tr}(\sigma_{i\neq\alpha}) = 0$

$$= \frac{\hbar}{4} \pi_\alpha \cdot 2$$

$$= \frac{\hbar}{2} \pi_\alpha .$$

The vector $\vec{\pi}$ is the polarization vector of the state. Measuring the components $\langle S_\alpha \rangle$ determines ρ. See (B) on page (7-8A)

Spin-1

$$S_x = \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \quad S_y = \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix} \quad S_z = \hbar \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

3 Dimensions

3-D vector: $\begin{pmatrix} a+ib \\ c+id \\ e+if \end{pmatrix} \rightarrow$ 6 parameters. (C)

1 phase is arbitrary $\Rightarrow$ 5 real params.

length = constant $\Rightarrow$ 4 real param.

3×3 ρ: (9 elements) 18 real parameters. (D)

9 conditions from Hermiticity.

a_{ii} = real

Re a_{ij} = Re a_{ji}

Im a_{ij} = − Im a_{ji}

$\therefore$ 9 net parameters, less 1 condition from trace.

2 Dimensions

2×2 ρ: 4 elements $\rightarrow$ 4 parameters after Hermiticity (B)

3 parameters after unit trace condition.

2-D vector $\begin{pmatrix} a+ib \\ c+id \end{pmatrix}$ 4 parameters (A)

less 1 since phase is arbitrary

less 1 constraint of fixed length

2 real parameters.

7-8B

(Insert half-way down pg. 7-9)

To fully determine ρ for $S=1$, we need a number of other measurements. These involve operators quadratic in S, namely $\hat{S}_\alpha \hat{S}_\beta + \hat{S}_\beta \hat{S}_\alpha$.

If we define

$$a_\alpha = \frac{\mathrm{Tr}(\hat{\rho}\hat{S}_\alpha)}{\hbar} \qquad \alpha = x, y, z$$

$$q_{\alpha\alpha} = \frac{\mathrm{Tr}(\hat{\rho}\hat{S}_\alpha^2)}{\hbar^2} \qquad \alpha = xx, yy \left(\begin{array}{l} zz \text{ determined} \\ \text{by } \mathrm{Tr}\,\rho = 1 \end{array}\right)$$

$$q_{\alpha\beta} = \frac{\mathrm{Tr}(\hat{\rho}(\hat{S}_\alpha\hat{S}_\beta + \hat{S}_\beta\hat{S}_\alpha))}{\hbar^2} \qquad \alpha\beta = xy, yz, zx.$$

It can be shown that

$$\rho = \begin{bmatrix} 1 + \frac{1}{2}(a_z - q_{xx} - q_{yy}) & \frac{1}{2\sqrt{2}}(a_x + q_{zx} - i(a_y + q_{yz})) & \frac{1}{2}(q_{xx} - q_{yy} - iq_{xy}) \\ \frac{1}{2\sqrt{2}}(a_x + q_{zx} + i(a_y + q_{yz})) & -1 + q_{xx} + q_{yy} & \frac{1}{2\sqrt{2}}(a_x - q_{zx} - i(a_y - q_{yz})) \\ \frac{1}{2}(q_{xx} - q_{yy} + iq_{xy}) & \frac{1}{2\sqrt{2}}(a_x - q_{zx} + i(a_y - q_{yz})) & 1 - \frac{1}{2}(a_z + q_{xx} + q_{yy}) \end{bmatrix}$$

How do we measure forms like $q_{\alpha\alpha}$ or $q_{\alpha\beta}$?

By definition: $\dfrac{\langle \hat{S}_\alpha^2 \rangle}{\hbar^2} = q_{\alpha\alpha}$ $\qquad \alpha = x, y.$ (2 measurements)

$$\frac{d}{dt}\langle \hat{S}_x^2 \rangle \bigg|_{\text{evaluated before } \rho \text{ changes.}} = \frac{i}{\hbar}\mathrm{Tr}\left(\hat{\rho}[\hat{H}, \hat{S}_x^2]\right)$$

use a uniform magnetic field with $\hat{H} = -\vec{\mu}\cdot\vec{B} \Rightarrow \hat{H} = \underset{\equiv c}{\underline{\text{const}}}\,\hat{S}_z$.

$$= \frac{i}{\hbar}\mathrm{Tr}\left(\hat{\rho}\,[c\hat{S}_z, \hat{S}_x^2]\right)$$

$$= -c\,\mathrm{Tr}\left(\hat{\rho}\,(\hat{S}_x\hat{S}_y + \hat{S}_y\hat{S}_x)\right)$$

$$= -c\hbar^2 q_{xy}.$$

$$[S_z, S_x^2] = S_z S_x S_x - S_x S_x S_z = i\hbar S_y S_x - (-i\hbar) S_x S_y = i\hbar(S_x S_y + S_y S_x)$$

The general set of eigenvectors pointing in the direction $\vec{n} = (\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta)$ is

$$\begin{array}{ccc} +1 & 0 & -1 \\ \begin{pmatrix} \frac{1}{2}(1+\cos\theta)e^{-i\varphi} \\ \frac{1}{\sqrt{2}}\sin\theta \\ \frac{1}{2}(1-\cos\theta)e^{i\varphi} \end{pmatrix} & \begin{pmatrix} -\sqrt{\frac{1}{2}}\sin\theta\, e^{-i\varphi} \\ \cos\theta \\ \sqrt{\frac{1}{2}}\sin\theta\, e^{i\varphi} \end{pmatrix} & \begin{pmatrix} \frac{1}{2}(1-\cos\theta)e^{-i\varphi} \\ -\sqrt{\frac{1}{2}}\sin\theta \\ \frac{1}{2}(1+\cos\theta)e^{i\varphi} \end{pmatrix} \end{array}.$$

See (C) on pg. (7-8A) Unlike $s = 1/2$, it is not true that every 3D vector (including complex phases) corresponds to an $s=1$ eigenstate. It takes 4 parameters to describe a 3D vector of fixed length, but only 2 parameters to describe $s=1$ state.

See (D) on page (7-8A) Further, measuring $\langle\vec{S}\rangle$ does not determine ρ. It takes 8 parameters to describe ρ, but $\langle\vec{S}\rangle$ provides only 3 constraints. [See page 7-8B for remaining conditions.]

Rotations

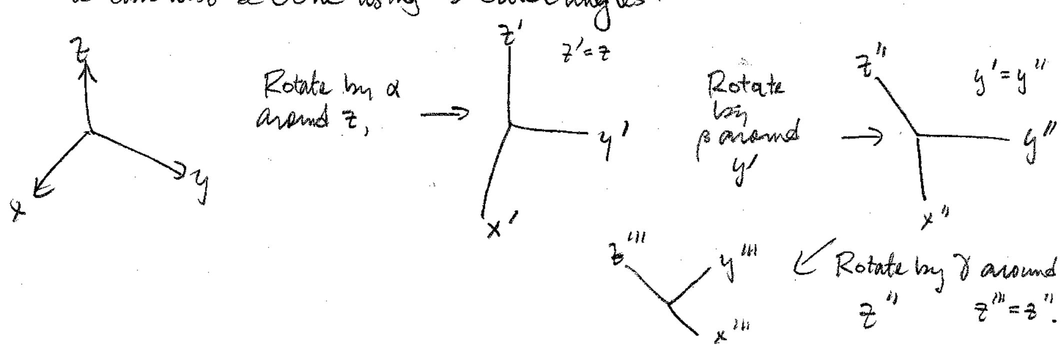
To describe a point in space at a given distance from the origin requires 2 parameters, θ, φ.

To describe a general rotation in space requires 3 parameters:

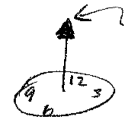
2 (θ, φ) to describe the axis

1 (φ') to describe the rotation around the axis.

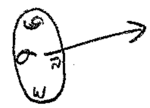
This can also be done using 3 Euler angles:



Aside: Think of describing the orientation of a disk



2 parameters to rotate normal to new position



Then another rotation on the face of the disk.

The Euler angles can be simplified by the following. As it stands, the Euler rotation is

$$\hat{R}(\alpha,\beta,\gamma) = e^{-i\gamma \hat{J}_{z''}}\, e^{-i\beta \hat{J}_{y'}}\, e^{-i\alpha \hat{J}_z} \qquad \left(\text{using } \hbar = 1\right).$$

But, from the transformation properties of operators, we know that:

$$\hat{J}_{y'} = \hat{R}_z(\alpha)\,\hat{J}_y\,\hat{R}_z(-\alpha) \quad \Rightarrow \quad e^{-i\beta \hat{J}_{y'}} = \hat{R}_{y'}(\beta)$$
$$= \hat{R}_z(\alpha)\,\hat{R}_y(\beta)\,\hat{R}_z(-\alpha).$$

And $\hat{R}_{z''}(\gamma) = \hat{R}_{y'}(\beta)\hat{R}_z(\alpha)\hat{R}_z(\gamma)\hat{R}_z(-\alpha)\hat{R}_{y'}(-\beta)$

$$\hat{J}_{z''} = \hat{R}_{y'}(\beta)\,\hat{J}_{z'}\,\hat{R}_{y'}(-\beta)$$
$$= \hat{R}_{y'}(\beta)\,\hat{R}_z(\alpha)\,\hat{J}_z\,\hat{R}_z(-\alpha)\,\hat{R}_{y'}(-\beta)$$

$$\Rightarrow R(\alpha,\beta,\gamma) = R_{z''}(\gamma)\,R_{y'}(\beta)\,R_z(\alpha)$$
$$= \left[R_{y'}(\beta)R_z(\alpha)R_z(\gamma)\underbrace{R_z(-\alpha)\underbrace{R_{y'}(-\beta)\right]\cdot R_{y'}(\beta)}_{=1}R_z(\alpha)}_{=1}$$

$$= R_{y'}(\beta)R_z(\alpha)R_z(\gamma)$$
$$= R_z(\alpha)R_y(\beta)R_z(-\alpha)R_z(\alpha)R_z(\gamma) = R_z(\alpha)R_y(\beta)R_z(\gamma).$$

Rotation Matrices

Suppose now that we want to take our state $|j\ m\rangle$ and rotate it using the rotation operator $\hat{R}(\alpha,\beta,\gamma)$. It is likely that the result

$$\hat{R}\,|jm\rangle$$

is of more interest to us if expressed in terms of the basis states $|jm\rangle$ as:

$$\hat{R}\,|jm\rangle = \sum_{j'm'} |j'\ m'\rangle \underbrace{\langle j'\ m'|\hat{R}\,|jm\rangle}$$

These coefficients are often written out in matrix form:

$$\langle j'm'|\,\hat{R}(\alpha,\beta,\gamma)\,|jm\rangle = \delta_{j'j}\, D^{(j)}_{m'm}(\alpha,\beta,\gamma).$$

Each matrix D depends on j.

The "matrix element" $\langle\ |R|\ \rangle$ is diagonal in j because $\hat{R}$ commutes with J^2. Reversing the definition:

$$D^{(j)}_{m'm}(\alpha,\beta,\gamma) = \langle j\ m'|\,e^{-i\alpha\hat{J}_z}\, e^{-i\beta\hat{J}_y}\, e^{-i\gamma\hat{J}_z}\,|jm\rangle \qquad (\hbar=1)$$

$$= e^{-i(\alpha m'+\gamma m)}\underbrace{\langle j\ m'|\,e^{-i\beta\hat{J}_y}\,|jm\rangle}_{\equiv\, d^{(j)}_{m'm}(\beta)}$$

$$\Rightarrow\ D^{(j)}_{m'm}(\alpha,\beta,\gamma) = e^{-i(\alpha m'+\gamma m)}\, d^{(j)}_{m'm}(\beta).$$

Let's work out some simple d's. $d^{(0)}_{m'm} = 1$

$j=1/2$: $\hat{J}$ ~~This~~ must have the matrix representation $\frac{1}{2}\hbar\vec{\underline{\sigma}}$

Pauli matrices.

Note: $3\,\sigma$'s for x,y,z, not $2\,\sigma$'s for $\uparrow\downarrow$

Now $\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$

$\begin{pmatrix}\text{Taking} \\ \hbar = 1\end{pmatrix} \Rightarrow e^{-\frac{i\beta}{2}\sigma_y} = e^{\frac{\beta}{2}\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}} = \mathbb{1} + \frac{\beta}{2}\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} + \frac{1}{2!}\left(\frac{\beta}{2}\right)^2\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \ldots$

$\left[\begin{array}{c}\text{or} \\ e^{-i\beta\hat{J}/\hbar} \\ = e^{-i\frac{\beta}{2}\sigma}\end{array}\right]$

$$= \mathbb{1}\cos\frac{\beta}{2} - i\sigma_y \sin\frac{\beta}{2}.$$

$$= \begin{pmatrix} \cos\frac{\beta}{2} & -\sin\frac{\beta}{2} \\ \sin\beta/2 & \cos\frac{\beta}{2} \end{pmatrix}$$

$$\equiv d^{1/2}_{m,m'}.$$

Note that this matrix is periodic in β with $\beta = 4\pi$. The matrix changes sign under rotation by 2π, a characteristic it shares with $j =$ odd integer $/2$.

By similar reasoning

$$d^{(1)}_{m'm} = \begin{pmatrix} \frac{1}{2}(1+\cos\beta) & -\frac{1}{\sqrt{2}}\sin\beta & \frac{1}{2}(1-\cos\beta) \\ \frac{1}{\sqrt{2}}\sin\beta & \cos\beta & -\frac{1}{\sqrt{2}}\sin\beta \\ \frac{1}{2}(1-\cos\beta) & \frac{1}{\sqrt{2}}\sin\beta & \frac{1}{2}(1+\cos\beta) \end{pmatrix}.$$

The spherical harmonics are related to the $\mathcal{D}$'s. Recall that the spherical harmonics $Y_{\ell m}(\theta,\varphi)$ are the coordinate representations of $|\ell\, m\rangle$ for integer ℓ, m. To find a relation between $\mathcal{D}$'s and Y's, we start with

R takes vector θ,φ to θ',φ'; R^{-1} takes $\psi(\theta,\varphi)$ to $\psi(\theta',\varphi')$

$$R^{-1}(\alpha,\beta,\gamma)\, Y_{\ell m}(\theta,\varphi) = Y_{\ell m}(\theta',\varphi') = \sum_{m'} Y_{\ell m'}(\theta,\varphi)\left(\mathcal{D}^{\ell}_{m'm}(\alpha,\beta,\gamma)\right)^{-1}$$

Since $\mathcal{D}$ is unitary, Inverse = complex transpose $\quad = \sum_{m'} Y \; \mathcal{D}^{\ell}_{mm'}(\alpha\beta\gamma)^*$

So, if we put $\beta = \gamma = 0$, then we have

$$R^{-1}(\alpha,0,0)\, Y_{\ell m}(\theta,\varphi) = \underbrace{R(0,0,-\alpha)}_{\substack{=R^{-1}(\alpha,0,0) \\ \text{from explicit} \\ \text{form of } R}}\, Y_{\ell m}(\theta,\varphi) = Y_{\ell m}(\theta, \varphi + \alpha) \quad ①$$

$$= \sum_{m'} Y_{\ell m'}(\theta,\varphi)\, D^{\ell}_{m m'}(\alpha,0,0)^*$$

$$= e^{i\alpha m}\, Y_{\ell m}(\theta,\varphi) \quad ②$$

$$\left[D^{\ell}_{m m'}(\alpha,0,0) = e^{-i\alpha m'} \cdot \delta_{m m'}\right]^*$$

Starting with

$$Y_{\ell m}(\theta',\varphi') = \sum_{m'} Y_{\ell m'}(\theta,\varphi)\left[D^{\ell}_{m m'}(\alpha,\beta,\gamma)\right]^*$$

we put $\theta = 0$ and $\varphi = 0$.

$$Y_{\ell m}(\beta,\alpha) = \sum_{m'} Y_{\ell m'}(0,0)\left[D^{\ell}_{m m'}(\alpha,\beta,0)\right]^*$$

Now, from ① + ② $Y_{\ell m}(\theta, \varphi+\alpha) = e^{i\alpha m}\, Y_{\ell m}(\theta,\varphi)$

If we put $\varphi = 0$, $Y_{\ell m}(\theta,\alpha) = e^{i\alpha m}\, Y_{\ell m}(\theta, 0)$.

But if $\theta = 0$, then the value of the spherical harmonic must be independent of α [polar vector is just pointing along z-axis]. This can only be true if

$m = 0 \quad Y_{\ell m}(0,0) \neq 0$

or $m \neq 0 \quad Y_{\ell m}(0,0) = 0$.

Hence, we write

$$Y_{\ell m}(0,0) = \underset{\text{some constant}}{c_\ell}\, \delta_{m,0}$$

$$Y_{\ell m}(\beta,\alpha) = \sum_{m'} c_\ell\, \delta_{m' 0}\left[D^{\ell}_{m m'}(\alpha,\beta,0)\right]^*$$

Conventionally one chooses $c_\ell = \left(\dfrac{2\ell+1}{4\pi}\right)^{1/2}$.

$$\Rightarrow Y_{\ell m}(\beta,\alpha) = c_\ell\left[D^{\ell}_{m 0}(\alpha,\beta,0)\right]^*$$