Representation of Rotation Matrices

- An arbitrary rotation is defined by the Euler angles α, β, γ

rotate α about z-axis
β " y'-axis (Goldstein uses x'!)
γ " z''-axis

Then $D(\alpha,\beta,\gamma) = e^{-i\gamma J_{z''}} e^{-i\beta J_{y'}} e^{-i\alpha J_z}$

The above is equivalent to
rotate γ about z-axis
β " y-axis
α " z-axis

Then $D(\alpha,\beta,\gamma) = e^{-i\alpha J_z} e^{-i\beta J_y} e^{-i\gamma J_z}$

Clearly $D^{-1}(\alpha,\beta,\gamma) = D(-\gamma,-\beta,-\alpha)$

D is obviously unitary so that $D^{-1}(R) = D^{\dagger}(R)$, where $R = \alpha,\beta,\gamma$.

- The set of $2j+1$ eigenvectors $|jm\rangle$, $m = j, j-1, \ldots, -j$ forms a basis set for a $2j+1$ dimensional irreducible representation of $D(R)$. The matrix elements are

$$\mathcal{D}^{j}_{m'm}(R) = \langle jm' | D(R) | jm \rangle$$

The group elements are $D(\alpha,\beta,\gamma)$ with α,β,γ being continuous labels.

- The unitarity condition $D^{\dagger} = D^{-1}$ implies that

$$[\mathcal{D}^{j}_{m^*m'}(\alpha,\beta,\gamma)]^* = \mathcal{D}^{j}_{m'm^*}(-\gamma,-\beta,-\alpha)$$

and $D^{\dagger}D = DD^{\dagger} = 1$ becomes, in matrix form

$$\sum_{m'} [\mathcal{D}^{j}_{m'n}(R)]^* \mathcal{D}^{(j)}_{m'm}(R) = \delta_{m,n}$$

<u>Evaluation of $\mathcal{D}^{j}_{m'm}(R)$</u>

$$\mathcal{D}^{j}_{m'm}(R) = \langle jm' | e^{-i\alpha J_z} e^{-i\beta J_y} e^{-i\gamma J_z} | jm \rangle$$

$$= e^{-i\alpha m' - i\gamma m} \underbrace{\langle jm' | e^{-i\beta J_y} | jm \rangle}_{d^{j}_{m'm}(\beta)}$$

$$d^{j}_{m'm}(\beta) = \sum_t \frac{(-1)^t [(j+m')!(j-m')!(j+m)!(j-m)!]^{1/2}}{(j+m'-t)!(j-m-t)!\,t!\,(t+m-m')!} \times \left(\cos\frac{\beta}{2}\right)^{2j+m'-m-2t} (\sin\beta/2)^{2t+m-m'}$$

Consequences.

~~The expression is unchanged by the interchange of m and m' together with the replacement of t by t + m' − m~~

i. Replace t by t + m' − m. Then

$$d^{j}_{m'm}(\beta) = (-1)^{m'-m} d^{j}_{mm'}(\beta)$$

Other symmetry relations:

$$d^{j}_{m'm}(\beta) = d^{j}_{-m,-m'}(\beta) = d^{j}_{m,m'}(-\beta)$$

$$= (-1)^{j-m'} d^{j}_{m',-m}(\pi - \beta)$$

<u>Special Values</u>

$$d^{j}_{m,n}(\pi) = (-1)^{j+m} \delta_{m,-n}$$

$$d^{j}_{m,n}(2\pi) = (-1)^{2j} \delta_{m,n}$$

For m = 0 $\mathcal{D}^{j}(\alpha, \beta, \gamma) = C^{*}(\beta, \alpha)$

Orthogonality

$$\int_0^{2\pi}\int_0^{2\pi}\int_0^{\pi}\left[\mathcal{D}^{j_1}_{m_1 m_1'}(\alpha\beta\gamma)\right]^* \mathcal{D}^{j_2}_{m_2 m_2'}(\alpha\beta\gamma)$$
$$\sin\beta\, d\beta\, d\alpha\, d\gamma$$

$$= \frac{8\pi^2}{2j_1+1}\,\delta_{m_1,m_2}\,\delta_{m_1',m_2'}\,\delta_{j_1,j_2}$$

The Case $j = 1/2$.

$$\underset{\sim}{J} = \frac{1}{2}\,\underset{\sim}{\sigma}$$

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\sigma_x^2 = \sigma_y^2 = \sigma_z^2 = \underset{\sim}{1}.$$

$$(\underset{\sim}{\sigma}\cdot\underset{\sim}{A})(\underset{\sim}{\sigma}\cdot\underset{\sim}{B}) = \underset{\sim}{A}\cdot\underset{\sim}{B} + i\,\sigma\cdot(\underset{\sim}{A}\times\underset{\sim}{B})$$ prove

$$(\underset{\sim}{\sigma}\cdot\underset{\sim}{n})^2 = \underset{\sim}{1}$$

$$(\underset{\sim}{\sigma}\cdot\underset{\sim}{n})^3 = (\sigma\cdot n)$$

$$(\sigma\cdot n)^{2j} = \underset{\sim}{1}, \quad (\underset{\sim}{\sigma}\cdot\underset{\sim}{n})^{2j+1} = (\sigma\cdot n)$$

$\therefore$ from power series expansion

$$e^{i\omega\underset{\sim}{\sigma}\cdot\underset{\sim}{n}} = \underset{\sim}{1}\cos\omega + i(\underset{\sim}{n}\cdot\underset{\sim}{\sigma})\sin\omega$$

$$\therefore\ e^{-i\beta J_y} = e^{-i\beta\sigma_y/2}$$

$$= \underset{\sim}{1}\cos\beta/2 - i\,\sigma_y\sin\beta/2$$

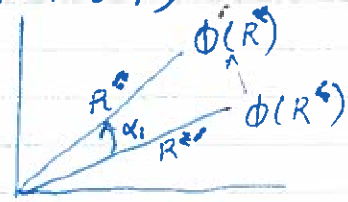
$$\therefore\ d^{1/2}_{mm'}(\beta) = \begin{pmatrix} \cos\beta/2 & -\sin\beta/2 \\ \sin\beta/2 & \cos\beta/2 \end{pmatrix}$$

The Rotation Matrices are Symmetric Top Eigenfcns.

.. Suppose an asymmetric rigid rotor has eigenfcn

$\phi(R)$, $R = \alpha, \beta, \gamma$ specifies orientation relative to z-axis. L_z is conserved and $\phi(R)$ is an eigenfcn of L_z and L^2.

If $\phi(R)$ is rotated ~~to~~ through $R_1 = (\alpha_1, \beta_1, \gamma_1)$ then the new fcn is



$$\phi'(R) = D(R_1)\phi(R) = \phi(R')$$

R' = ~~point~~ axis carried into R by rotation R_1

If $\phi(R) = \phi_{IN}(R)$ is an eigenfcn of L^2, L_z, H, then $\phi'(R)$ is a linear combination of $\phi_{IM}(R)$, $M = -I, \dots, I$.

$$\phi'(R) = \sum_M \phi_{IM}(R) \langle IM | D(R_1) | IN \rangle$$

$$= \sum_M \phi_{IM}(R) \mathcal{D}^I_{MN}(R_1) = \phi_{IN}(R')$$

If $R_1 = R = (\alpha, \beta, \gamma)$, then $R' = (0,0,0)$

$$\phi'(R) = \sum_M \phi_{IM}(R) \mathcal{D}^I_{MN}(R) = \Phi_{IN}(0)$$

$$\sum_N \mathcal{D}_{M_1N}^* \left(\qquad \right)$$

$$\phi_{IM_1}(R) = \sum_N \mathcal{D}^*_{M_1N}(R) \phi_{IN}(0)$$

∴ general form of asymmetric rigid rotor eigenfcn. M_1 = angular mom. component about z-axis.

If in addition L_z' = symmetry axis, then a rotation through arbitrary angle γ about z' axis should leave wave fcn invariant (up to a phase)

$$\mathcal{D}^{I}_{MN}(R) = e^{-i(\alpha M + \gamma N)}\, d^{I}_{MN}(\beta)$$

∴ only one N value contributes.

$\mathcal{D}^{I*}_{MN}(R)$ is simultaneous eigenfcn of L_z, L_z' with eigenvalues M, $+N$.

Use of Rotation Matrices

- Suppose an atom has a set of eigenstates $|JN\rangle$ of J_z and a set of axes (x', y', z') is obtained by a rotation R from (x, y, z). The eigenstates $|JN\rangle'$ of J_z' are obtained from $|JN\rangle$ by

$$|JN\rangle' = D(R)\,|JN\rangle$$

$$= \sum_M |JM\rangle\langle JM|D(R)|JN\rangle$$

$$= \sum_M |JM\rangle\, \mathcal{D}^{J}_{MN}(R)$$

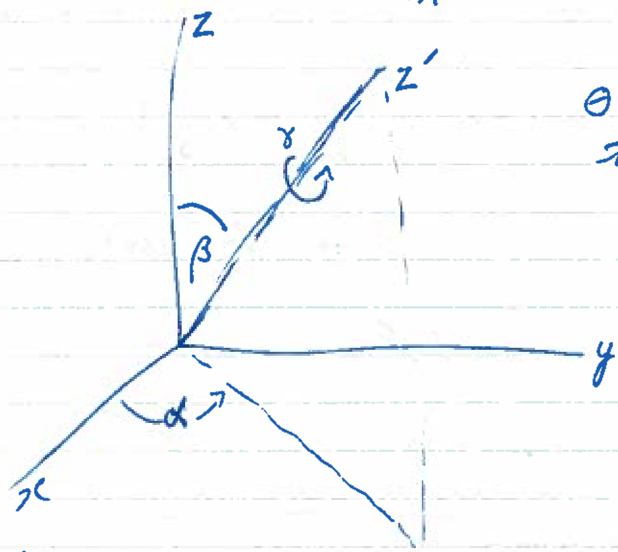
- States which transform as above are said to transform cogradiently. The dual states

$$'\langle JN| = \langle JN|D^{\dagger} = \sum_M \mathcal{D}^{J*}_{MN} \langle JM|$$

transform contragradiently.

Example - spherical harmonics

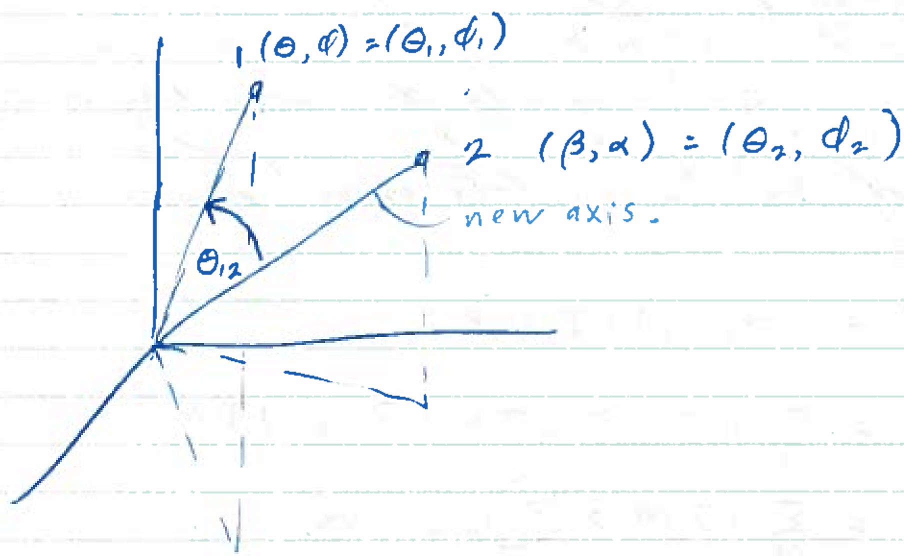
$$C_{ln}(\theta', \phi') = \sum_m \mathcal{D}^{l}_{mn}(\alpha, \beta, \gamma)\, C_{lm}(\theta, \phi)$$



θ', φ' are angles relative to x', y', z' axes.

If $n = 0$,

$$P_l(\cos\theta') = \sum_m C^*_{lm}(\beta, \alpha)\, C_{lm}(\theta, \phi)$$

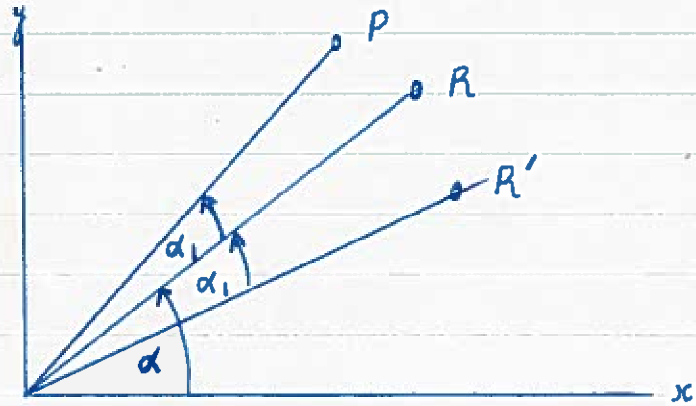


$$P_l(\cos\theta_{12}) = \frac{4\pi}{2l+1} \sum_m Y_l^m(\theta_2, \phi_2)^* \, Y_l^m(\theta_1, \phi_1)$$

Rotation conventions and Notation.

1. A positive (counter clockwise) rotation refers to a positive rotation of the system. This is equivalent to a negative rotation of the co-ordinate axes.

2. Let the system be rotated through angle α_1 about the z-axis. The wave function $\Phi(\alpha)$ rotates with the system.



A point R in the system rotates with the system to the point P, while the direction R' rotates into R.

Call the rotated wave function $\Phi'(\alpha)$.

Then $\Phi'(P) = \Phi(R)$

i.e. $\Phi'(\alpha+\alpha_1) = \Phi(\alpha)$.

$\therefore \quad \Phi'(\alpha) = \Phi(\alpha - \alpha_1)$

or $\quad \Phi'(R) = \Phi(R')$

3. $D(\alpha_1)$ is the rotation operator which relates $\Phi'(R)$ to $\Phi(R)$ such that

$$\Phi'(R) = D(\alpha_1)\,\Phi(R).$$

If $\alpha_1 = \alpha$, then R' coincides with the x-axis and thus

$$\underline{\Phi}'(R) = D(\alpha)\underline{\Phi}(R) = \underline{\Phi}(0). \qquad (1)$$

$$\therefore \underline{\Phi}(R) = D^{-1}(\alpha)\underline{\Phi}(0).$$

4. Rigid Rotor Eigenfunctions

- Let $\Phi_{LM}(R)$ be a simultaneous eigenfunction of L^2, L_z. Then from (1)

$$D(R)\underline{\Phi}_{LM}(R) = \underline{\Phi}_{LM}(0)$$

$$\therefore \underline{\Phi}_{LM}(0) = \sum_{M'} \mathcal{D}^L_{M';M}(R)\,\underline{\Phi}_{LM'}(R)$$

Using the unitarity of the $\mathcal{D}$ matrices, this can be transformed to

$$\underline{\Phi}_{LM}(R) = \sum_{M'} \mathcal{D}^{L\,*}_{M,M'}(R)\,\underline{\Phi}_{LM'}(0). \qquad (2)$$

This is the most general form for a simultaneous eigenfunction of L^2, L_z. The spherical harmonics correspond to the single term with $M' = 0$.

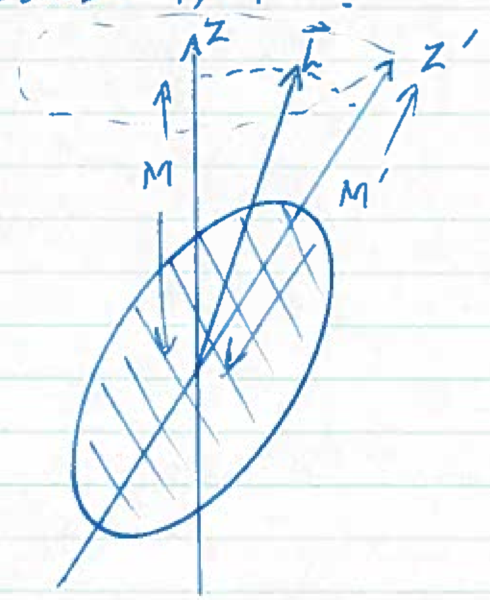
$\Phi_{LM}(R)$ can be interpreted as the general form of an asymmetric rigid rotor eigenfunction. M = angular momentum component about z'-axis.

If in addition the z' body-fixed axis is also a symmetry axis, then a rotation through an arbitrary angle γ about z' should leave the wave function invariant (up to a phase).

But $\mathcal{D}^{L}_{MM'}(R) = e^{-i(\alpha M + \gamma M')} d^{L}_{MM'}(\beta)$

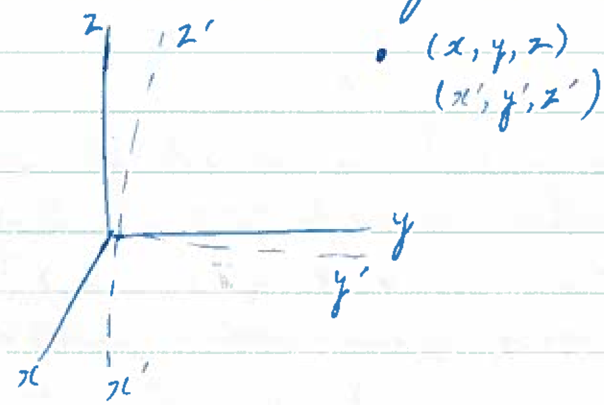
$\therefore$ only one M' value contributes.

Thus $\mathcal{D}^{L}_{MM'}(R)$ is a simultaneous eigenfunction of L_z and $L_{z'}$ with eigenvalues M, M'.



Question - How can two components of $\vec{L}$ be simultaneously quantized? ie L_z and $L_{z'}$.

Answer - If the primed axes were fixed wrt the unprimed axes, then L_z and $L_{z'}$ could not be simultaneously quantized. However the primed axes rotate rigidly with the symmetric top.



$$L_z = \frac{1}{i}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) \qquad (x', y', z' \text{ fixed})$$

$$= \frac{1}{i}\frac{\partial}{\partial \alpha}$$

$$L_{z'} = \frac{1}{i}\left(x'\frac{\partial}{\partial y'} - y'\frac{\partial}{\partial x'}\right) \qquad (x, y, z \text{ fixed})$$

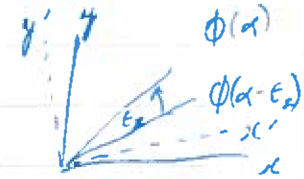
$$= +\frac{1}{i}\frac{\partial}{\partial \gamma}$$

and $[L_z, L_{z'}] = 0$.

To see the above, consider

$$D(R_1)\,\phi(R) = \phi(R')$$

For a rotation through ϵ_z about the z-axis is



$$\phi'(\alpha,\beta,\gamma) = (1 - i\epsilon_z L_z)\,\phi(\alpha,\beta,\gamma) \simeq \phi(\alpha-\epsilon_z, \beta, \gamma)$$

$$\simeq \phi(\alpha,\beta,\gamma) - \epsilon_z \frac{\partial\phi}{\partial\alpha}$$

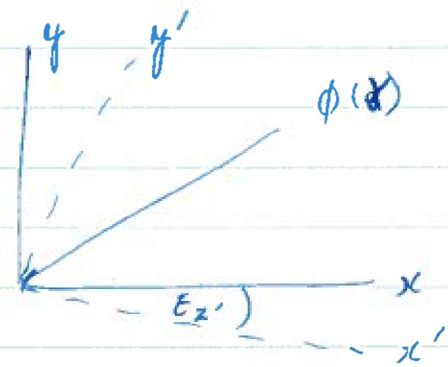
$$\therefore\ L_z = -i\frac{\partial}{\partial\alpha}$$

Since (x', y', z') are held fixed, the primed axes rotate with the body. The final orientation is $\phi(\alpha \mp \epsilon_z, \beta, \gamma)$.

- Consider now the rotation generated by $L_{z'}$ (x, y, z) fixed. The orientation of the body is changed in the "body-fixed" co-ordinate system.

$$\phi'(\alpha,\beta,\gamma) = (1 - i\epsilon_{z'} L_{z'})\,\phi(\alpha,\beta,\gamma) \simeq \phi(\alpha,\beta,\gamma \mp \epsilon_{z'})$$

$$\simeq \phi(\alpha,\beta,\gamma) \mp \epsilon_{z'}\frac{\partial\phi}{\partial\gamma}$$



$$\therefore\ L_{z'} = -i\frac{\partial}{\partial\gamma}$$

Since the final orientation is unchanged in the space-fixed axes, the Euler angles are