

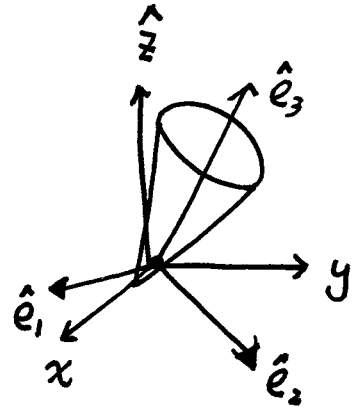
Lect 1 D-matrix as rotation wavefunctions - spinning top

Let us consider a rigid rotor, how to describe its rotation wavefunction in a quantum mechanical way? Physically, this can be a molecule, Now, we are quantizing the motion of a top.

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The configuration space of a top can be denoted by the Eulerian angles (α, β, γ) .

The relation between the body frame (e_1, e_2, e_3) and the lab frame (x, y, z) is



$$(\hat{e}_1, \hat{e}_2, \hat{e}_3) = (x, y, z) \begin{pmatrix} \cos\alpha \cos\beta \cos\gamma - \sin\alpha \sin\gamma & -\cos\alpha \cos\beta \sin\gamma - \sin\alpha \cos\gamma & \cos\alpha \sin\beta \\ \sin\alpha \cos\beta \cos\gamma + \cos\alpha \sin\gamma & -\sin\alpha \cos\beta \sin\gamma + \cos\alpha \cos\gamma & \sin\alpha \sin\beta \\ -\sin\beta \cos\gamma & \sin\beta \sin\gamma & \cos\beta \end{pmatrix}$$

$T(\alpha, \beta, \gamma)$

SO(3) matrix. - special orthogonal matrix.

Ex: prove the above relation following the definition of Eulerian angles (α, β, γ) . Check the rotation matrices for x, y, z -axes.

Hint:

and perform the matrix product.

The angular momenta in the Lab frame is defined as

L_x, L_y, L_z , which are conserved quantities, and we will prove it later. Q_1, Q_2, Q_3 are angular momentum components projections

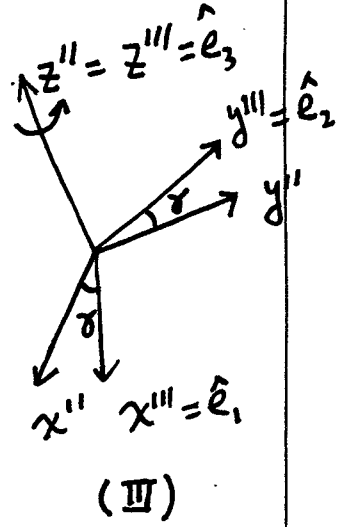
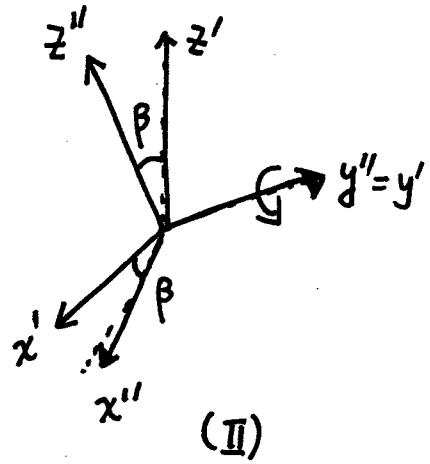
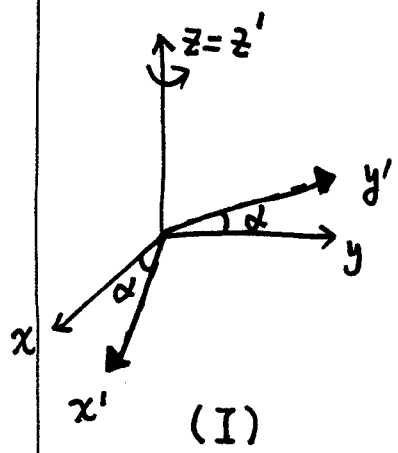
on e_1, e_2 and e_3 axes. We know that from classic mechanics

$$H = \frac{Q_1^2}{2I_1} + \frac{Q_2^2}{2I_2} + \frac{Q_3^2}{2I_3} \quad (\text{a free top, no external torque}).$$

Next we derive the expressions of $L_{x,y,z}$ and $Q_{1,2,3}$ in terms of

α, β, γ . According to the definition,

$$\hat{L}_z = -i\hbar \frac{\partial}{\partial \alpha}, \quad \hat{Q}_3 = -i\hbar \frac{\partial}{\partial \gamma}$$



According to (II), $\hat{L}_{y'} = -i\hbar \frac{\partial}{\partial \beta}$, and $\hat{y}' = \cos\alpha \hat{y} - \sin\alpha \hat{x}$

$$\Rightarrow \cos\alpha \hat{L}_y - \sin\alpha \hat{L}_x = \hat{L}_{y'} = -i\hbar \frac{\partial}{\partial \beta} \quad (*)$$

$$\hat{z}'' = \cos\beta \hat{z} + \sin\beta \hat{x}' = \cos\beta \hat{z} + \sin\beta (\cos\alpha \hat{x} + \sin\alpha \hat{y})$$

$$\Rightarrow \hat{L}_{z''} = \hat{Q}_3 = -i\hbar \frac{\partial}{\partial r} = \cos\beta \hat{L}_z + \sin\beta \cos\alpha \hat{L}_x + \sin\beta \sin\alpha \hat{L}_y$$

$$\Rightarrow \cos\alpha \hat{L}_x + \sin\alpha \hat{L}_y = -\frac{i\hbar}{\sin\beta} \frac{\partial}{\partial r} + \cot\beta i\hbar \frac{\partial}{\partial \alpha} \quad (**)$$

from (*) and (**), we arrive at

$$\hat{L}_x = -i\hbar \left[-\cos\alpha \cot\beta \frac{\partial}{\partial \alpha} - \sin\alpha \frac{\partial}{\partial \beta} + \frac{\cos\alpha}{\sin\beta} \frac{\partial}{\partial r} \right]$$

$$\hat{L}_y = -i\hbar \left[-\sin\alpha \cot\beta \frac{\partial}{\partial \alpha} + \cos\alpha \frac{\partial}{\partial \beta} + \frac{\sin\alpha}{\sin\beta} \frac{\partial}{\partial r} \right]$$

Similarly $\hat{e}_1 = \hat{x}''' = \hat{x}'' \cos\gamma + \hat{y}'' \sin\gamma = (\cos\beta \hat{x}' - \sin\beta \hat{z}') \cos\gamma + \hat{y}' \sin\gamma$

$$\Rightarrow \hat{Q}_1 = \cos\beta \underbrace{[\cos\alpha \hat{x} + \sin\alpha \hat{y}]}_{\cos\gamma} - \sin\beta \cos\gamma \hat{z}' + \hat{y}' \sin\gamma$$

$$\hat{Q}_1 = \cos\beta \underbrace{[\cos\alpha \hat{L}_x + \sin\alpha \hat{L}_y]}_{\cos\gamma} - \sin\beta \cos\gamma \hat{L}_z - i\hbar \frac{\partial}{\partial \beta} \sin\gamma$$

$$\hat{Q}_1 = -i\hbar \left[\sin\gamma \frac{\partial}{\partial \beta} - \frac{\cos\gamma}{\sin\beta} \frac{\partial}{\partial \alpha} + \cot\beta \cos\gamma \frac{\partial}{\partial r} \right]$$

$$\hat{e}_2 = \hat{y}''' = -\sin\gamma \hat{x}'' + \cos\gamma \hat{y}'$$

$$= -\sin\gamma [\cos\beta \hat{x}' - \sin\beta \hat{z}'] + \cos\gamma \hat{y}'$$

$$= -\sin\gamma \cos\beta [\cos\alpha \hat{x} + \sin\alpha \hat{y}] + \sin\gamma \sin\beta \hat{z}' + \cos\gamma \hat{y}'$$

$$\Rightarrow \hat{Q}_2 = -\sin\gamma \cos\beta [\cos\alpha \hat{L}_x + \sin\alpha \hat{L}_y] + \sin\gamma \sin\beta \hat{L}_z - \cos\gamma i\hbar \frac{\partial}{\partial \beta}$$

$$\Rightarrow Q_1 = -i\hbar \left[-\frac{\cos\gamma}{\sin\beta} \frac{\partial}{\partial\alpha} + \sin\gamma \frac{\partial}{\partial\beta} + \cot\beta \cos\gamma \frac{\partial}{\partial\gamma} \right]$$

$$Q_2 = -i\hbar \left[\frac{\sin\gamma}{\sin\beta} \frac{\partial}{\partial\alpha} + \cos\gamma \frac{\partial}{\partial\beta} - \cot\beta \sin\gamma \frac{\partial}{\partial\gamma} \right]$$

Ex: check that $Q_i = (\hat{e}_i \cdot \vec{L}) = \hat{\chi}_{ij}^T (\alpha \beta \gamma) \cdot \vec{L}$

$$\Rightarrow Q_i = T_{ij} (\alpha \beta \gamma) \hat{L}_j$$

Since $Q_i = (\hat{e}_i \cdot \vec{L})$, under rotations, both \hat{e}_i and \vec{L} transform in the same way and thus keep the inner product invariant.

In other words, Q_i is a scalar under rotation. \Rightarrow

$$D^\dagger(\varphi) Q_i D(\varphi) = Q_i, \text{ or } e^{i\vec{L} \cdot \hat{n} \theta} Q_i e^{-i\vec{L} \cdot \hat{n} \theta} = Q_i$$

$$\Rightarrow [L_j, Q_i] = 0$$

The Lab frame angular momentum and body frame ones commute!

Ex: please check $[L_j, Q_i] = 0$ from their expressions using (α, β, γ) by brutal force calculation.

For a free top, we have $[L^2, H] = [L_z, H] = [L^2, L_z] = 0$, thus

we can choose (L^2, L_z) to characterize the rotation eigenstate of a top.

However, we know that (L^2, L_z) is complete for a point particle confined on a sphere, but a top is more than a single particle. Later, we will see that we need an extra quantum number.

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Now let us denote the wavefunction $\psi_{IM}(g)$, where IM are the quantum numbers for L^2, L_z , respectively. The configuration space of a top is characterized

by (α, β, γ) , which determines an $SO(3)$ rotation, i.e. the rotation from the lab frame (xyz) to the body frame (e_1, e_2, e_3) . $\widehat{g(\alpha\beta\gamma)}$ Thus the configuration space of a top is the same as the group space of $SO(3)$. We will use "g" as the coordinate of rotating top.

Let us apply the rotation g_0 on the wavefunction $\psi_{IM}(g)$.

$$R(g_0) \psi_{IM}(g) = \psi_{IM}(g_0^{-1}g)$$

↑ rotation
 ↑ coordinate of the configuration space of top
 ← product according to group operation

on the other hand,

$$R(g_0) \psi_{IM}(g) = \sum_{M'} \psi_{IM'}(g) D_{M'M}^I(g_0)$$

Let set $g_0 = g \Rightarrow \psi_{IM}(e) = \sum_{M'} \psi_{IM'}(g) D_{M'M}^I(g) = \sum_{M'} (D_{MM'}^I)^T \psi_{IM'}(g)$

$$\psi_{IM}(g) = \sum_{M'} (D^{I, T})_{MM'}^\dagger(g) \psi_{IM'}(e) = \sum_{M'} D_{M, M'}^{*, I}(g) \psi_{IM'}(e)$$

Before we move on, let's define the ~~orthogonal~~ ^{orthogonal} conditions of $D_{MM'}^{*, I}(g)$.

① measure $\int dg = \int_0^{2\pi} d\alpha \int_0^\pi \underbrace{d\beta}_{\sin\beta} \int_0^{2\pi} d\gamma = 8\pi^2$

$$D_{m'_1 m_1}^{I_1}(g) = \langle I_1, m'_1 | D(g) | I_1, m_1 \rangle, \quad D_{m'_2 m_2}^{I_2}(g) = \langle I_2, m'_2 | D(g) | I_2, m_2 \rangle$$

Theorem: $\int dg D_{m'_1 m_1}^{I_1, *}(g) D_{m'_2 m_2}^{I_2}(g) = C(I_1) \delta_{I_1, I_2} \delta_{m'_1 m'_2} \delta_{m_1 m_2}$, and

$$C(I_1) = \frac{8\pi^2}{2I_1 + 1}$$

Proof: define an operator $P = \int dg D^\dagger(g) |I_1, m'_1\rangle \langle I_2, m'_2| D(g)$

where $D(g) = e^{-i \vec{J} \cdot \hat{n} \theta}$

let us define a rotation g_0 , and $P \rightarrow \cancel{P} \rightarrow P' = D^\dagger(g_0) P D(g_0)$

~~$P = \int dg D^\dagger(g) |I_1, m'_1\rangle \langle I_2, m'_2| D(g)$~~

$$P' = \int dg D^\dagger(g_0) D^\dagger(g) |I_1, m'_1\rangle \langle I_2, m'_2| D(g) D(g_0)$$

$$= \int dg D^\dagger(g g_0) |I_1, m'_1\rangle \langle I_2, m'_2| D(g g_0)$$

$$= \int d(g' g_0) D^\dagger(g') |I_1, m'_1\rangle \langle I_2, m'_2| D(g') = \int dg D^\dagger(g) |I_1, m'_1\rangle \langle I_2, m'_2| D(g)$$

↑
measure is invariant

$$= P$$

then $\int dg D_{m_1 m_1}^{I_1*}(g) D_{m_2 m_2}^{I_2}(g) = \langle I_1 m_1 | P | I_2 m_2 \rangle$

since P is rotationally invariant $\Rightarrow \int dg D_{m_1 m_1}^{I_1*}(g) D_{m_2 m_2}^{I_2}(g) \propto \delta_{I_1 I_2} \delta_{m_1 m_2}$

similarly $\Rightarrow \propto \delta_{m_1 m_1}$

The result is also only dependent on I_1 , but not m 's. ~~...~~
i.e. $C(I_1)$

$$\Rightarrow C(I_1) = \frac{1}{2I_1+1} \sum_{m_1} \int D_{m_1 m_1}^{* I_1}(g) D_{m_1 m_1}^{I_1}(g) dg$$

$$= \frac{1}{2I_1+1} \sum_{m_1} \int \left[D_{m_1 m_1}^{I_1}(g) \right]^\dagger D_{m_1 m_1}^{I_1}(g) dg = \frac{1}{2I_1+1} \int dg = \frac{8\pi^2}{2I_1+1}$$

$$\Rightarrow \int D_{m_1 m_1}^{I_1*}(g) D_{m_2 m_2}^{I_2}(g) dg = \frac{8\pi^2}{2I_1+1} \delta_{I_1 I_2} \delta_{m_1 m_1} \delta_{m_2 m_2}$$

Now we can interpret $D_{MM'}^{*,I}(g)$ as the basis of rotation functions of a top. We also know that IM are not complete to describe top. we can assign m' as another quantum number to classify bases.

orth-normal basis (IMM')

$$\psi_{IMM'}(g) = \sqrt{\frac{2I+1}{8\pi^2}} D_{MM'}^{*,I}(g)$$

Next, we need to figure out what is the physical meaning of the quantum number of M' .

by definition, we apply rotation on top wavefunction

$$e^{-i\theta \hat{n} \cdot \vec{J}} \psi(g) = \psi(g^{-1}(\hat{n}, \theta) \cdot g)$$

Replace $\psi(g) = D_{MM'}^{I,*}(\alpha \beta \gamma)$, where $g = g(\alpha \beta \gamma) \Rightarrow$

$$e^{-i\theta \hat{n} \cdot \vec{J}} D_{MM'}^{I,*}(\alpha \beta \gamma) = \left[D_{MM'}^I(g_0^{-1}(\hat{n}, \theta) g) \right]^* \\ = \sum_{M''} D_{MM''}^{I,*}(g_0^{-1}(\hat{n}, \theta)) D_{M''M'}^{I,*}(g) = \sum_{M''} D_{M''M'}^{I,*}(g) D_{M'',M}^I(g_0(\hat{n}, \theta))$$

→ take infinitesimal rotation, and remember $g = g(\alpha \beta \gamma)$

$$\hat{n} \cdot \vec{J} D_{MM'}^{I,*}(\alpha \beta \gamma) = \sum_{M''} D_{M'',M'}^{I,*}(\alpha \beta \gamma) \langle IM'' | \hat{n} \cdot \vec{J} | IM \rangle$$

operation on the first m-index.

now take \hat{n} to be one of the top body axes, $\hat{e}_{k=1,2,3}$

$$\hat{e}_k = g(\alpha \beta \gamma) \hat{i}_k \quad \hat{i}_k = \hat{x}, \hat{y}, \hat{z}; \text{ the fixed frame axis.}$$

$$\hat{Q}_k = \hat{e}_k \cdot \vec{J} \Rightarrow Q_k D_{MM'}^{I,*}(\alpha \beta \gamma) = \sum_{M''} D_{M'',M'}^{I,*}(\alpha \beta \gamma) \langle IM'' | \hat{e}_k \cdot \vec{J} | IM \rangle$$

$$\hat{e}_k \cdot \vec{J} = \vec{J} \cdot g(\alpha \beta \gamma) \hat{i}_k = (g^{-1} \vec{J}) \cdot \hat{i}_k = D(g) (\vec{J} \cdot \hat{i}_k) D(g)^{-1}$$

$$\Rightarrow \langle IM'' | Q_k | IM \rangle = \sum_{K'K''} \langle IM'' | D(g) | IK' \rangle \langle IK' | \vec{J} \cdot \hat{i}_k | IK'' \rangle \langle IK'' | D(g)^{-1} | IM \rangle$$

$$= \sum_{K',K''} D_{M''K'}^I(g) D_{K''M}^I(g^{-1}) \langle IK' | J_k | IK'' \rangle$$

$$Q_k D_{MM'}^{I,*}(\alpha\beta\gamma) = \sum_{\substack{M'' \\ K'K''}} D_{M''M'}^{I,*}(\alpha\beta\gamma) D_{M'',K'}^I(g) D_{K''M}^I(g^{-1}) \langle IK' | J_k | IK'' \rangle$$

Sum over M''

$$\sum_{M''} D_{M''M'}^{I,*}(\alpha\beta\gamma) D_{M''K'}^I(\alpha\beta\gamma) = \delta_{K'M'}$$

$$\begin{aligned} \Rightarrow Q_k D_{MM'}^{I,*}(\alpha\beta\gamma) &= \sum_{K''} D_{K''M}^I(g^{-1}) \langle IM' | J_k | IK'' \rangle \\ &= \sum_{K''} D_{MK''}^{I,*}(g) \langle IM' | J_k | IK'' \rangle \end{aligned}$$

set $k=3 \Rightarrow \langle IM' | J_z | IK'' \rangle = \delta_{M'K''} M'$

$$\Rightarrow \boxed{Q_3 D_{MM'}^{I,*} = M' D_{MM'}^{I,*}} \leftarrow M' \text{ is the eigen-number of } Q_3.$$

more generally \Rightarrow

$$\boxed{(\vec{J} \cdot \hat{e}_k) D_{MM'}^{I,*}(\alpha\beta\gamma) = \sum_{M''} D_{M''M'}^{I,*}(\alpha\beta\gamma) \langle IM' | \vec{J} \cdot \hat{e}_k | IM'' \rangle}$$

operations on ~~the second index in the lower line~~
the second m-index.