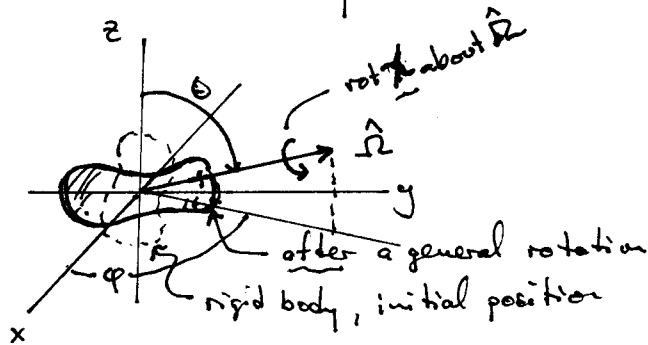


Rotations & Rot. matrices in QM

pp. 1-6
 (from Rose, Elem. Thy. of Ang. Mom.)

Rotations of a rigid body in 3D require 3 parameters to completely specify a specific rot R .

Intuitively these are angles (θ, φ) to give the new orientation of the original body-fixed \hat{z} axis, and an angle α that gives the rotation of the body itself about the new \hat{z} direction:



two equivalent choices in the description

- "body-fixed coord system" moves with the body.
- "space-fixed coord system" does not change.

Many choices for the three rigid-body angles are possible. The most often used in classical and quantum mechanics are the "Euler angles" (α, β, γ) .

definition: ^{1st, recall:} a general rotation about an axis \hat{n} by θ in QM is given by

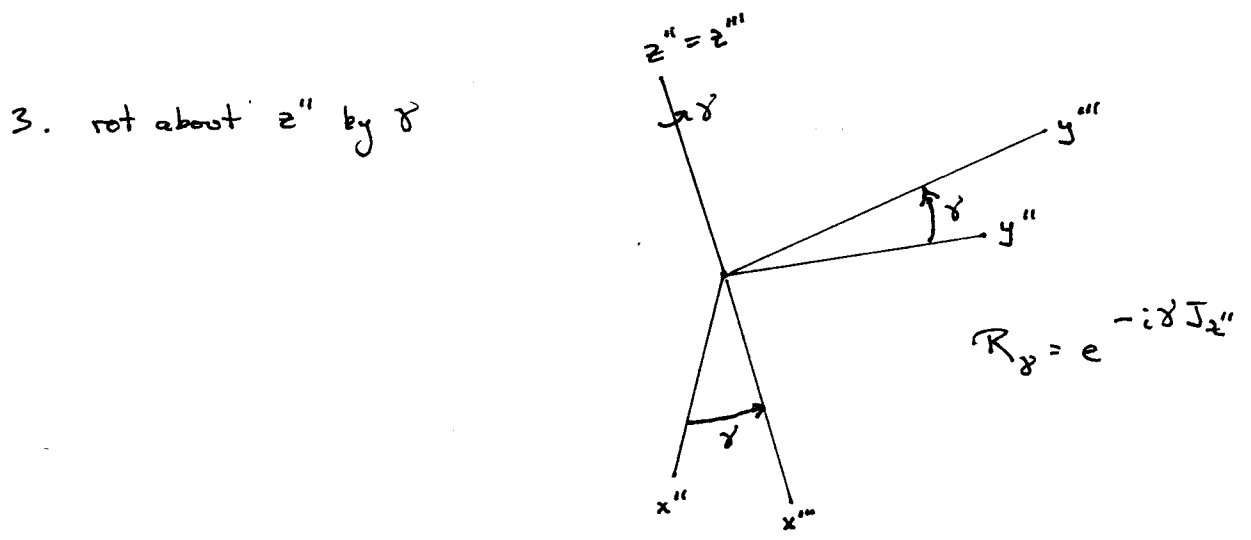
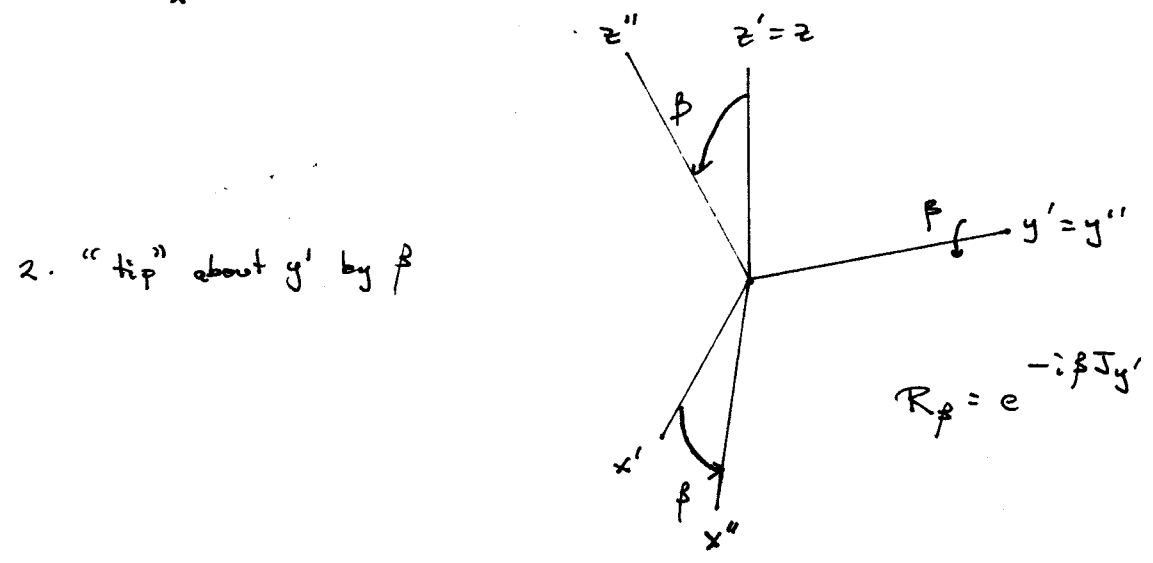
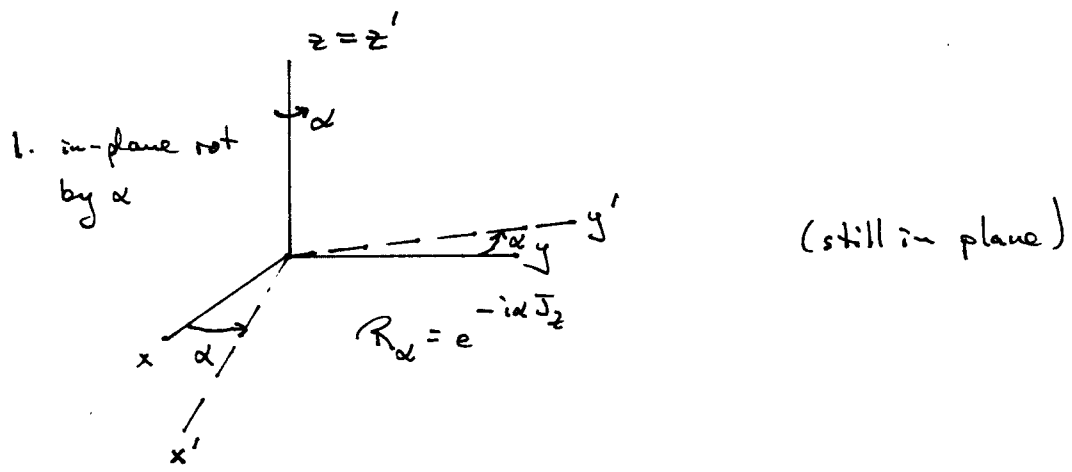
$$U(\theta \hat{n}) = e^{-i\theta \hat{n} \cdot \vec{J}}$$

suppose we define the rot. by a three-stage transformation of the coordinate system:

1) rot. about \hat{z} by α $R_\alpha = e^{-i\alpha J_z}$

2) rot. about the new \hat{y}' axis by β $R_\beta = e^{-i\beta J_{y'}}$

3) finally, rot. about the \hat{z}'' axis by γ $R_\gamma = e^{-i\gamma J_{z''}}$



Looks complicated, more so than (θ, ϕ, ψ) , but it's easier to calculate with

$$R = \underbrace{e^{-i\gamma J_{z''}}}_{R_\gamma} \underbrace{e^{-i\beta J_{y'}}}_{R_\beta} \underbrace{e^{-i\alpha J_z}}_{R_\alpha}$$

1st simplification: we can ^{simply} relate these ' and '' coordinate rotations to rotations about the original x y z axes.

The rot. by β about y' , $e^{-i\beta J_{y'}}$, is the same as

1. rot back to the original coord sys ($-\alpha$)
2. rot about the original y axis by β
3. return rot to the new coordinate sys (α)

So,

$$\underbrace{e^{-i\beta J_{y'}}}_{R_\beta \text{ about } y'} = \underbrace{e^{-i\alpha J_z}}_{3. R_{+\alpha} \text{ about } z} \underbrace{e^{-i\beta J_y}}_{2. R_\beta \text{ about } y} \underbrace{e^{i\alpha J_z}}_{1. R_{-\alpha} \text{ about } z}$$

Similarly, the rot by δ about z'' can be "backed up" to a rotation by δ about the previous z' ,

$$\underbrace{e^{-i\delta J_{z''}}}_{R_\delta \text{ about } z''} = \underbrace{e^{-i\beta J_{y'}}}_{3. R_\beta \text{ about } y'} \underbrace{e^{-i\delta J_{z'}}}_{2. R_\delta \text{ about } z'} \underbrace{e^{i\beta J_{y'}}}_{1. R_{-\beta} \text{ about } y'}$$

which gives

$$R_{\alpha\beta\delta} = \underbrace{\left(e^{-i\beta J_{y'}} e^{-i\delta J_{z'}} e^{i\beta J_{y'}} \right)}_{R_\delta} \underbrace{e^{-i\beta J_{y'}}}_{R_\beta} \underbrace{e^{-i\alpha J_z}}_{R_\alpha}$$

$$= \left(e^{-i\alpha J_z} e^{-i\beta J_y} e^{i\alpha J_z} \right) \underbrace{e^{-i\delta J_{z'}}}_{\left(e^{-i\alpha J_z} e^{-i\delta J_{z'}} e^{i\alpha J_z} \right)} e^{-i\beta J_y}$$

$$\therefore \underline{R_{\alpha\beta\delta} = e^{-i\alpha J_z} e^{-i\beta J_y} e^{-i\delta J_z}}$$

Thus the original rotation \equiv three rotations about space-fixed axes, if the order of rot. is inverted. Much easier for QM!

Rotation matrices

Now we can evaluate the effect of a general rotation $R_{\alpha\beta\gamma}$ on a quantum state $|jm\rangle$. Since total angular momentum \vec{J}^2 is conserved under rotations, we expect a linear combination of $\{|jm'\rangle\}$ basis states.

This defines the "rotation matrix" (Wigner)

$$R_{\alpha\beta\gamma} |jm\rangle \equiv \sum_{m'} d_{m'm}^{(j)}(\alpha, \beta, \gamma) |jm'\rangle$$

The coefficients that make up the rotation matrix can "easily" be evaluated as matrix elements,

$$d_{m'm}^{(j)}(\alpha, \beta, \gamma) = \langle jm' | R_{\alpha\beta\gamma} | jm \rangle = \langle jm' | e^{-i\alpha J_z} e^{-i\beta J_y} e^{-i\gamma J_z} | jm \rangle$$

$$= \underbrace{e^{-i\alpha m'} e^{-i\beta m}}_{\text{simple phases for rot. about } z} \underbrace{\langle jm' | e^{-i\beta J_y} | jm \rangle}_{\text{nontrivial m.e.s.}}$$

$$\equiv d_{m'm}^{(j)}(\beta)$$

these are real polynomials in $\cos(\beta/2)$ and $\sin(\beta/2)$

Wigner gives the d-functions as a series,

$$d_{m'm}^{(j)}(\beta) = \left[\frac{(j+m)!(j-m)!(j+m')!(j-m')!}{(j+m-k)!(j+m-k)!(k+m'-m)!k!} \right]^{1/2} \cdot \sum_k \frac{(-1)^k}{\cos(\beta/2)^{2j+m-n-2k} \sin(\beta/2)^{m'-m+2k}} \quad (m' \geq m)$$

where the integer k runs over all values for which the factorials are nonsingular (≥ 0).

It may not help to know that this can be written as a ${}_2F_1$ hypergeometric function,

$$d_{m'm}^{(j)}(\beta) = \left[\frac{(j-m)!(j+m')!}{(j+m)!(j-m')!} \right]^{1/2} \frac{\cos\left(\frac{\beta}{2}\right)^{2j+m-m'} \left(-\sin\left(\frac{\beta}{2}\right)\right)^{m'-m}}{(m'-m)!}$$

$$\cdot {}_2F_1\left(m'-j, -m-j; m'-m+1; -\tan^2\left(\frac{\beta}{2}\right)\right)$$

there is also a closed-form result involving Jacobi polynomials

$$(m' \geq m)$$

n.b.

$${}_2F_1(a, b; c; x) = \sum_{n=0}^{\infty} \frac{(a)_n (b)_n x^n}{(c)_n n!}$$

$$(a)_n \equiv a(a+1) \dots (a+n-1)$$

$$\text{and } (0)_0 \equiv 1$$

Some simple properties of the d-functions and examples

$$\left. \begin{aligned} d_{m'm}^{(j)}(-\beta) &= (-1)^{m'-m} d_{m'm}^{(j)}(\beta) \\ d_{m'm}^{(j)}(-\beta) &= d_{mm'}^{(j)}(\beta) \end{aligned} \right\} \Rightarrow \underline{d_{m'm}^{(j)}(\beta) = (-1)^{m'-m} d_{mm'}^{(j)}(\beta)}$$

↳ This is because a rot by $-\beta$ gives the transpose of the $+\beta$ rot. matrix.
 (inverse rot, $R_{-\beta} = R_{\beta}^{-1}$) (matrices) $(R^T = R^{-1})$

the closed form result implies

$$\underline{d_{m'm}^{(j)}(\beta) = d_{-m, -m'}^{(j)}(\beta)}$$

$$\underline{d_{m'm}^{(j)}(\beta) = (-1)^{m'-m} d_{-m', -m}^{(j)}(\beta)}$$

(can use this for $m' < m$ on ${}_2F_1$ formula above)

Simple properties from defⁿ of rots:

Note for

$$R_{\alpha\beta\gamma} = e^{-i\alpha J_z} e^{-i\beta J_y} e^{-i\gamma J_z}$$

the inverse rotation is simply

$$R_{\alpha\beta\gamma}^{-1} = e^{+i\gamma J_z} e^{+i\beta J_y} e^{+i\alpha J_z}$$

and since $\mathcal{D}^\dagger = \mathcal{D}^{-1}$,

$$\langle j m' | R_{\alpha\beta\gamma}^{-1} | j m \rangle = \langle j m | R_{\alpha\beta\gamma} | j m' \rangle^*$$

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

$$e^{+im'\gamma} e^{+im\alpha} \mathcal{D}_{m'm}^{(j)}(-\beta) = e^{+i\alpha m} e^{+i\gamma m'} \mathcal{D}_{mm'}^{(j)}(\beta)$$

which was given previously

Products of rotation matrices $\mathcal{D} \cdot \mathcal{D}$

These arise e.g. when we consider rotations of composite states. Recall from the CG series for a product state

$$|j, m\rangle = \sum_{m_1, m_2} \underbrace{\langle j_1, m_1, j_2, m_2 | j, m \rangle}_{\text{CG coeffs}} |j_1, m_1\rangle |j_2, m_2\rangle$$

Now suppose we apply a general $R_{\alpha\beta\gamma}$ rotation to this state:

$$\begin{aligned} \underline{R_{\alpha\beta\gamma} |j, m\rangle} &= \sum_{m'} \mathcal{D}_{m'm}^{(j)}(\alpha, \beta, \gamma) |j, m'\rangle \\ &= \sum_{\substack{m_1, m_2 \\ m', m_2'}} \langle j_1, m_1, j_2, m_2 | j, m \rangle R_{\alpha\beta\gamma} \{ |j_1, m_1\rangle |j_2, m_2\rangle \} \\ &= \sum_{\substack{m_1, m_2 \\ m', m_2'}} \langle j_1, m_1, j_2, m_2 | j, m \rangle \mathcal{D}_{m_1' m_1}^{(j_1)}(\alpha, \beta, \gamma) \mathcal{D}_{m_2' m_2}^{(j_2)}(\alpha, \beta, \gamma) |j_1, m_1'\rangle |j_2, m_2'\rangle \end{aligned}$$

Pull out the 1^{st} rotation matrix by multiplying by $\langle j, m'' |$, (α relabel $m'' \rightarrow m'$);

$$\begin{aligned} \rightarrow \mathcal{D}_{m'm}^{(j)}(\alpha, \beta, \gamma) &\equiv R = \sum_{\substack{m_1, m_2 \\ m', m_2'}} \langle j_1, m_1, j_2, m_2 | j, m \rangle \mathcal{D}_{m_1' m_1}^{(j_1)}(R) \mathcal{D}_{m_2' m_2}^{(j_2)}(R) \\ &\quad \underbrace{\langle j, m' | |j_1, m_1'\rangle |j_2, m_2'\rangle}_{\text{itself the CG coeff}} \\ &\quad \langle j, m' | j_1, m_1', j_2, m_2' \rangle \end{aligned}$$

or

$$\mathcal{D}_{m'm}^{(j)}(R) = \sum_{\substack{m_1, m_2 \\ m', m_2'}} \langle j_1, m_1, j_2, m_2 | j, m \rangle \langle j, m' | j_1, m_1', j_2, m_2' \rangle \cdot \mathcal{D}_{m_1' m_1}^{(j_1)}(R) \mathcal{D}_{m_2' m_2}^{(j_2)}(R)$$

note really only a double sum: $m_2 = m - m_1$, $m_2' = m' - m_1'$

This can be used to construct all higher- j rot. matrices e.g. starting from $j_1, j_2 = 1/2$!

since the magnetic phases are trivial, this is really an identity for the nontrivial d-functions

$$d_{m'm}^{(j)}(\beta) = e^{-i\alpha m'} e^{-i\delta m} \underline{d_{m'm}^{(j)}(\beta)}$$

an e.g. Let's try it and see. what is $d_{00}^{(1)}(\beta)$?

$$\underline{d_{00}^{(1)}(\beta)} = \sum_{\substack{m_1, m_2 \\ m_1', m_2'}} \langle 1/2 m_1, 1/2 m_2 | 10 \rangle \langle 10 | 1/2 m_1', 1/2 m_2' \rangle d_{m_1' m_1}^{(1/2)}(\beta) d_{m_2' m_2}^{(1/2)}(\beta)$$

n.b.

$$|10\rangle = \frac{1}{\sqrt{2}} |1/2 1/2\rangle |1/2 -1/2\rangle + \frac{1}{\sqrt{2}} |1/2 -1/2\rangle |1/2 1/2\rangle$$

∴ all CG coeffs shown here are $\pm 1/\sqrt{2}$.

$$\begin{aligned} &= \underbrace{\langle 1/2 1/2, 1/2 -1/2 | 10 \rangle^2}_{1/2} \cdot \frac{d_{1/2 1/2}^{(1/2)}(\beta)}{e} \frac{d_{-1/2 -1/2}^{(1/2)}(\beta)}{e} && c \equiv \cos(\beta/2) \\ &+ \underbrace{\langle 1/2 -1/2, 1/2 1/2 | 10 \rangle^2}_{1/2} \cdot \frac{d_{-1/2 -1/2}^{(1/2)}(\beta)}{e} \frac{d_{1/2 1/2}^{(1/2)}(\beta)}{e} && \Delta \equiv \sin(\beta/2) \\ &+ \underbrace{\langle 1/2 1/2, 1/2 -1/2 | 10 \rangle \cdot \langle 10 | 1/2 -1/2, 1/2 1/2 \rangle}_{1/2} \cdot \frac{d_{-1/2 1/2}^{(1/2)}(\beta)}{\Delta} \cdot \frac{d_{1/2 -1/2}^{(1/2)}(\beta)}{-\Delta} \\ &+ \underbrace{\langle 1/2 -1/2, 1/2 1/2 | 10 \rangle \cdot \langle 10 | 1/2 1/2, 1/2 -1/2 \rangle}_{1/2} \cdot \frac{d_{1/2 -1/2}^{(1/2)}(\beta)}{-\Delta} \cdot \frac{d_{-1/2 1/2}^{(1/2)}(\beta)}{\Delta} \\ &= \frac{1}{2} \{ 2e^2 - 2\Delta^2 \} = \cos^2(\beta/2) - \sin^2(\beta/2) = \underline{\cos(\beta)} \quad \checkmark \end{aligned}$$

Can similarly build up all higher $d_{m'm}^{(j)}(\beta)$ functions, given the CG coefficients and $\{d_{m'm}^{(1/2)}(\beta)\}$.

Opposite direction: rot. of $|j_1\rangle |j_2\rangle$ states

$$\underline{|j_1 m_1\rangle |j_2 m_2\rangle = \sum_{j m (m=m_1+m_2)} \langle j m | j_1 m_1, j_2 m_2 \rangle |j m\rangle}$$

apply a general rotation $R_{\alpha\beta\gamma}$

$$\underline{R \{ |j_1 m_1\rangle |j_2 m_2\rangle \}} = \sum_{m'_1 m'_2} d_{m'_1 m_1}^{(j_1)}(R) d_{m'_2 m_2}^{(j_2)}(R) |j_1 m'_1\rangle |j_2 m'_2\rangle$$

$$= \sum_{\substack{j m m' \\ \underbrace{}_{=m_1+m_2, \text{ not really a sum}}} \langle j m | j_1 m_1, j_2 m_2 \rangle d_{m' m}^{(j)}(R) |j m'\rangle$$

dot $\langle j_1 m'_1 | \langle j_2 m'_2 |$ into this equation, (then reset " \rightarrow ');

$$\underline{d_{m'_1 m_1}^{(j_1)}(R) d_{m'_2 m_2}^{(j_2)}(R)}$$

$$= \sum_{\substack{j m m' \\ \underbrace{}_{=m'_1+m'_2 \\ m_1+m_2} \text{ not really summed}}} \langle j m | j_1 m_1, j_2 m_2 \rangle d_{m' m}^{(j)}(R) \underbrace{\langle j_1 m'_1 | \langle j_2 m'_2 |}_{\text{CG coeff}} |j m'\rangle$$

$$= \sum_{\substack{j \\ \underbrace{}_{\text{only real sum}}}} \langle j m | j_1 m_1, j_2 m_2 \rangle \langle j_1 m'_1, j_2 m'_2 | j m' \rangle \underbrace{d_{m' m}^{(j)}(R)}_{\text{fixed}}$$

Thus the product of two rotation matrices, in general of different spin, the entries of can be written as a sum of individual $d_{m' m}^{(j)}$ matrices, with a sum over j , from $|j_1 - j_2|$ to $j_1 + j_2$.

This is the CG series for rotation matrices.

What use is this decomposition to us?

One surprising result: Gaunt formula!

Recall for integer l we stated

$$D_{m0}^{(l)}(\alpha, \beta, \gamma) = \left(\frac{4\pi}{2l+1}\right)^{1/2} Y_{lm}^*(\beta, \alpha)$$

This implies, from prev $D \cdot D$ result,

$$\begin{aligned}
D_{m'_1 0}^{(l_1)}(\alpha, \beta, \gamma) D_{m'_2 0}^{(l_2)}(\alpha, \beta, \gamma) &= \frac{4\pi}{\sqrt{(2l_1+1)(2l_2+1)}} Y_{l_1 m'_1}^*(\beta, \alpha) Y_{l_2 m'_2}^*(\beta, \alpha) \\
&= \sum_l \langle l m | l_1 0, l_2 0 \rangle \cdot \langle l_1 m'_1, l_2 m'_2 | l m \rangle \underbrace{D_{m'_1 0}^{(l)}(\alpha, \beta, \gamma)}_{\left(\frac{4\pi}{2l+1}\right)^{1/2} Y_{lm}^*(\beta, \alpha)}
\end{aligned}$$

$$\begin{aligned}
\therefore \frac{Y_{l_1 m_1}(\alpha) \cdot Y_{l_2 m_2}(\alpha)}{\sqrt{4\pi}} &= \frac{1}{\sqrt{4\pi}} \sum_l \left[\frac{(2l_1+1)(2l_2+1)}{(2l+1)} \right]^{1/2} \\
&\quad \leftarrow (|l_1 - l_2| \text{ to } l_1 + l_2) \\
&\quad \cdot \langle l 0 | l_1 0, l_2 0 \rangle \cdot \langle l_1 m_1, l_2 m_2 | l m \rangle \\
&\quad \cdot \frac{Y_{lm}(\alpha)}{\sqrt{4\pi}} \quad \leftarrow l = m_1 + m_2
\end{aligned}$$

This is the Gaunt formula, which was given w/o justification previously.

Dynamical application - rotational levels of a rigid body in QM (~ molecules)

The classical Hamiltonian for rot. of a rigid body is

$$H = \sum_{i=1}^3 \frac{L_i^2}{2I_i}$$

↑
princ. axes = a, b, c
→ (always an orthogonal set)

For the QM version, factor an \hbar out of each ang. mom. op. & we have

$$H_{op} = \sum_{i=1}^3 \frac{\hbar^2}{2I_i} \hat{L}_i^2$$

special cases are the spherically symmetric top $I_a = I_b = I_c = I$

axially symm top $I_a = I_b = I, I_c = I' \neq I$

and asymm top, all different.

The 1st two cases are easy to solve in QM.

Note: the angular momentum operators $\{\hat{L}_i\}$ refer to body-fixed coordinates (= rots. about a, b, c body-fixed axes).

The work is in rewriting these ops. in space-fixed coordinates, such as the Euler angles (α, β, γ) , or our original set (θ, ϕ, χ) .

In the latter coords this gives, for the axisymmetric top (Pauling + Wilson)

$$H_{op} = -\frac{\hbar^2}{2I} \left\{ \frac{1}{\sin^2 \theta} \partial_\theta (\sin^2 \theta \partial_\theta) + \frac{1}{\sin^2 \theta} \partial_\phi^2 + \left(\frac{1}{\tan^2 \theta} + \frac{I}{I'} \right) \partial_\chi^2 - \frac{2 \cos \theta}{\sin^2 \theta} \partial_{\chi\phi}^2 \right\}$$

& we are to find a wavefunction $\underline{\Psi(\theta, \phi, \chi)}$ that satisfies

$$\underline{H_{op} \Psi = E \Psi.}$$

→ orientation amplitude
This will give the spectrum of states for the asymm. rigid rotator.

by inspection, the magnetic angles are plane waves,

$$\Psi(\theta, \varphi, x) = e^{im\varphi} e^{ikx} \cdot f_{m,k}(\theta)$$

integers, each 0, ±1, ±2, ...

$$-\frac{\hbar^2}{2I} \left\{ f'' + \cot(\theta) f' - \frac{m^2}{\sin^2(\theta)} f - \left(\frac{I}{I'} + \frac{1}{\tan^2(\theta)} \right) f + \frac{2mk \cos(\theta)}{\sin^2(\theta)} f \right\} = E f$$

$$' = \frac{d}{d\theta}$$

the solution of this DE is $f = d_{m,k}^{(\ell)}(\theta)$,

and the resulting energies are

$$\Psi(\theta, \varphi, x) = \eta e^{im\varphi} e^{ikx} d_{m,k}^{(\ell)}(\theta)$$

(not normalized yet)

$$E = \frac{\hbar^2}{2I} \ell(\ell+1) + \frac{\hbar^2}{2} (I'^{-1} - I^{-1}) k^2$$

This can be seen more intuitively using

$$H = \frac{\hbar^2}{2I} (\hat{L}_a^2 + \hat{L}_b^2) + \frac{\hbar^2}{2I'} \hat{L}_c^2 = \frac{\hbar^2}{2I} \underbrace{\hat{L}^2}_{\substack{\text{also } \hat{L}^2 \\ \text{space-fixed,} \\ \ell(\ell+1) \text{ eigenvalue}}} + \frac{\hbar^2}{2} (I'^{-1} - I^{-1}) \underbrace{\hat{L}_c^2}_{\substack{k^2 \text{ on } e^{ikx}}}$$

$$\therefore E = \frac{\hbar^2}{2I} \ell(\ell+1) + \frac{\hbar^2}{2} \left(\frac{1}{I'} - \frac{1}{I} \right) k^2 \text{ is expected anyway!}$$