Representation of Rotation and Spherical Harmonics

Nov. 29, 2016

ClassEval due by Dec. 5 (M) 8am
Final Exam : Dec. 8 (Thursday) 8-11am

Euler rotation

$$R(\alpha,\beta,\gamma) = R_{z''}(\gamma)\, R_{y'}(\beta)\, R_z(\alpha)$$
$$= R_z(\alpha)\, R_y(\beta)\, R_z(\gamma)$$

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

Hilbert Space Rotation ; Drehung

$$\mathcal{D}(\alpha,\beta,\gamma) = e^{\frac{-iJ_z\alpha}{\hbar}}\, e^{\frac{-iJ_y\beta}{\hbar}}\, e^{\frac{-iJ_z\gamma}{\hbar}}$$

Matrix elements of $\mathcal{D}(\alpha,\beta,\gamma)$ define the Wigner function, representing the rotation operator in Hilbert space.

$$\langle j, m' | \mathcal{D}(\alpha,\beta,\gamma) | j, m\rangle \equiv \mathcal{D}^{(j)}_{m'm}(\alpha,\beta,\gamma)$$

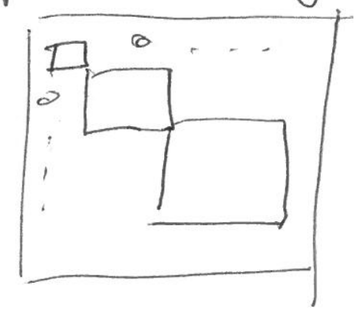
$$= \langle j, m' | e^{\frac{-iJ_z\alpha}{\hbar}}\, e^{\frac{-iJ_y\beta}{\hbar}}\, e^{\frac{-iJ_z\gamma}{\hbar}} | j, m\rangle$$

$$= e^{-i(m'\alpha + m\gamma)} \underbrace{\langle j, m' | e^{\frac{-iJ_y\beta}{\hbar}} | j, m\rangle}_{d^{(j)}_{m',m}(\beta)}$$

(nontrivial part)

$\boxed{(2j+1)\times(2j+1) \text{ matrix}}$

(2j+1)-dimensional irreducible representation of the rotation operator $\mathcal{D}(R)$



e.g. For spin-$\frac{1}{2}$ system ; $J_y = \frac{\hbar}{2}\sigma_y$

$$d^{(\frac{1}{2})}(\beta) = e^{-i\sigma_y \frac{\beta}{2}} = \cos\frac{\beta}{2} - i\sigma_y \sin\frac{\beta}{2} \doteq \begin{array}{cc} m=+ & m=- \\ \left[\begin{array}{cc} \cos\frac{\beta}{2} & -\sin\frac{\beta}{2} \\ \sin\frac{\beta}{2} & \cos\frac{\beta}{2} \end{array}\right] & \begin{array}{l} m'=+ \\ m'=- \end{array} \end{array}$$

$$d^{(\frac{1}{2})}(\beta)|+\rangle = \sum_{m'} |m'\rangle \underbrace{\langle m'| d^{(\frac{1}{2})}(\beta)|+\rangle}_{d^{(\frac{1}{2})}_{m'+}(\beta)}$$

$$= \cos\frac{\beta}{2}|+\rangle + \sin\frac{\beta}{2}|-\rangle$$

For $\beta = \pi$,
$d^{(\frac{1}{2})}(\pi)|+\rangle = |-\rangle$

For spin-1 system.

$$d^{(1)}(\beta) = e^{\frac{-iJ_y\beta}{\hbar}} = I - i\frac{J_y}{\hbar}\sin\beta - \left(\frac{J_y}{\hbar}\right)^2(1-\cos\beta)$$

$$\doteq \begin{bmatrix} 1 & & 0 \\ & 1 & \\ 0 & & 1 \end{bmatrix} - \frac{i}{\hbar}\left(\frac{i\hbar}{\sqrt{2}}\right)\begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix}\sin\beta - \frac{1}{\cancel{\hbar^2}}\frac{\cancel{\hbar^2}}{2}\begin{bmatrix} 1 & 0 & -1 \\ 0 & 2 & 0 \\ -1 & 0 & 1 \end{bmatrix}(1-\cos\beta)$$

$\sin^2\frac{\beta}{2}$

$$= \begin{bmatrix} \frac{1+\cos\beta}{2} & -\frac{\sin\beta}{\sqrt{2}} & \frac{1-\cos\beta}{2} \\ \frac{\sin\beta}{\sqrt{2}} & \cos\beta & -\frac{\sin\beta}{\sqrt{2}} \\ \frac{1-\cos\beta}{2} & \frac{\sin\beta}{\sqrt{2}} & \frac{1+\cos\beta}{2} \end{bmatrix} = \begin{bmatrix} \cos^2\frac{\beta}{2} & -\sqrt{2}\sin\frac{\beta}{2}\cos\frac{\beta}{2} & \sin^2\frac{\beta}{2} \\ \sqrt{2}\sin\frac{\beta}{2}\cos\frac{\beta}{2} & \cos^2\frac{\beta}{2}-\sin^2\frac{\beta}{2} & -\sqrt{2}\sin\frac{\beta}{2}\cos\frac{\beta}{2} \\ \sin^2\frac{\beta}{2} & \sqrt{2}\sin\frac{\beta}{2}\cos\frac{\beta}{2} & \cos^2\frac{\beta}{2} \end{bmatrix}$$

$\cos^2\frac{\beta}{2}$ $\quad -\sqrt{2}\sin\frac{\beta}{2}\cos\frac{\beta}{2}$

In general for any j, Wigner's formular for $d^{(j)}_{m',m}(\beta)$ is given by Eq. (3.9.33), p. 238

$$d^{(j)}_{m',m}(\beta) = \sum_k (-1)^{k-m+m'} \frac{\sqrt{(j+m)!\,(j-m)!\,(j+m')!\,(j-m')!}}{(j+m-k)!\,k!\,(j-k-m')!\,(k-m+m')!} \times \left(\cos\frac{\beta}{2}\right)^{2j-2k+m-m'} \left(\sin\frac{\beta}{2}\right)^{2k-m+m'}$$

Schwinger's derivation in <u>Section 3.9</u> using creation and annihilation operators in the system of two <u>uncoupled</u> harmonic oscillator model:

$$\text{Spin-}\tfrac{1}{2} \begin{cases} \uparrow \text{ — } +\text{type oscillator} \\ \downarrow \text{ — } -\text{type oscillator} \end{cases} \longrightarrow \boxed{\begin{array}{l} J_+ \equiv \hbar a_+^\dagger a_- \\ J_- \equiv \hbar a_-^\dagger a_+ \end{array}}$$

$$|j,m\rangle = \frac{(a_+^\dagger)^{j+m}(a_-^\dagger)^{j-m}}{\sqrt{(j+m)!\,(j-m)!}}|0\rangle \qquad \text{e.g. } |1,0\rangle = \cancel{a_+^\dagger a_-^\dagger|0\rangle}$$

<u>Ex</u>. Consider an orbital angular momentum eigenstate $|l=1, m=0\rangle$. Suppose this state is rotated by an angle β about y-axis. Find the probability for the new state to be found in $m=+1, 0, -1$ states,

$$d^{(1)}(\beta)\,|\,l=1,\ m=0\rangle$$

$$= \sum_{m'=-1}^{+1} |\,l=1,\ m'\rangle \underbrace{\langle l=1,\ m'\,|\,d^{(1)}(\beta)\,|\,l=1,\ m=0\rangle}_{d^{(1)}_{m'0}(\beta)}$$

$$\begin{array}{cc} \begin{bmatrix} d^{(1)}_{11} & \boxed{\begin{matrix} d^{(1)}_{10} \\ d_{00} \\ d_{-10} \end{matrix}} & d^{(1)}_{1-1} \\ & & \\ & & \end{bmatrix} & \begin{matrix} m'=1 \\ m'=0 \\ m'=-1 \end{matrix} \\ \begin{matrix} m=+1 & \quad m=0 & \quad m=-1 \end{matrix} & \end{array}$$

$$= -\frac{\sin\beta}{\sqrt{2}}\,|1,1\rangle + \cos\beta\,|1,0\rangle + \frac{\sin\beta}{\sqrt{2}}\,|1,-1\rangle$$

Note

1) Probability sum is 1 as it must be.

$$P_{m'=\pm 1} = \frac{\sin^2\beta}{2}, \quad P_{m'=0} = \cos^2\beta \quad \left(\sum_{m'=-1}^{+1} P_{m'} = 1\right)$$

2) Correspondence to the Spherical Harmonics:

Eq. (B.5.7) p.528

$$Y_1^{\pm 1}(\theta,\phi) = \mp\sqrt{\frac{3}{8\pi}}\sin\theta\, e^{\pm i\phi}$$

$$Y_1^{0}(\theta,\phi) = \sqrt{\frac{3}{4\pi}}\cos\theta$$

$$d^{(1)}(\beta)\,|1,0\rangle = \sqrt{\frac{4\pi}{3}}\left(Y_1^{1*}(\beta,0)\,|1,1\rangle + Y_1^{0*}(\beta,0)\,|1,0\rangle + Y_1^{-1*}(\beta,0)\,|1,-1\rangle\right)$$

Note more general formula: Eq. (3-6.52) p.206

$$\mathcal{D}^{(l)}_{m0}(\alpha,\beta,\gamma=0) = \sqrt{\frac{4\pi}{2l+1}}\,Y_l^{m*}(\beta,\alpha)$$

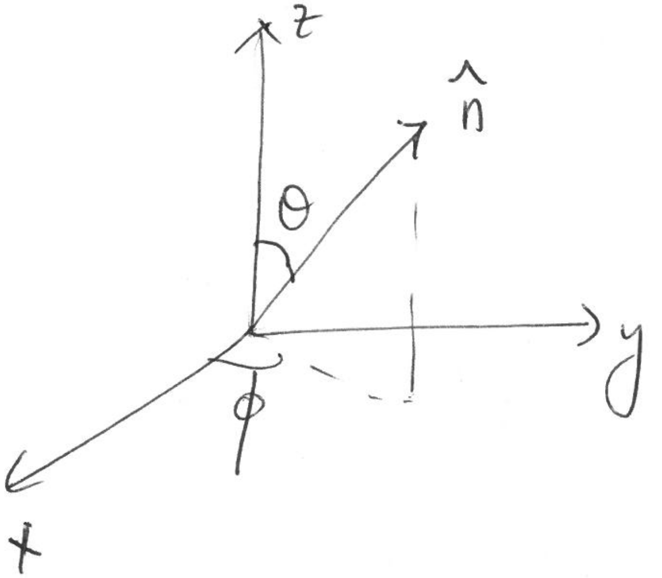
What is spherical Harmonics?

How can we prove Eq. (3.6.52)?

Spherical Harmonics is the <u>spherical coordinate representation of the orbital angular momentum eigenstates</u>.

$|l,m\rangle$; i.e.

$$Y_l^m(\theta,\phi) \equiv \langle\theta,\phi|l,m\rangle = \langle\hat{n}|l,m\rangle = Y_l^m(\hat{n}).$$



$$|\underset{\substack{\uparrow \\ \beta}}{\theta},\underset{\substack{\uparrow \\ \alpha}}{\phi}\rangle = |\hat{n}\rangle$$

$$|\hat{n}\rangle = \mathcal{R}(\alpha=\phi,\ \beta=\theta,\ \gamma=0)\,|\hat{z}\rangle$$

$$= \sum_{l,m} \mathcal{D}(\alpha=\phi,\ \beta=\theta,\ \gamma=0)\,|l,m\rangle\langle l,m|\hat{z}\rangle$$

$$\underbrace{\langle l,m'|\hat{n}\rangle}_{Y_l^{m'*}(\hat{n})} = \sum_m \mathcal{D}^{(l)}_{m'm}(\phi,\theta,0)\,\underbrace{\langle l,m|\hat{z}\rangle}_{Y_l^{m*}(\theta=0,\ \phi\ \text{undetermined})}$$

$\uparrow \delta_{m0}$

$$Y_\ell^{m'*}(\hat{n}) = \sum_m \mathcal{D}^{(\ell)}_{m'm}(\phi,\theta,0)\, \underbrace{Y_\ell^{m*}(\theta=0, \phi \text{ undetermined})}_{\substack{\| \\ \sqrt{\frac{2\ell+1}{4\pi}}\, P_\ell(\cos\theta=1)\,\delta_{m,0} \\ \| \\ \sqrt{\frac{2\ell+1}{4\pi}}\,\delta_{m,0}}}$$

$$= \mathcal{D}^{(\ell)}_{m'0}(\phi,\theta,0)\sqrt{\frac{2\ell+1}{4\pi}}$$

$$\text{or } \mathcal{D}^{(\ell)}_{m'0}(\phi,\theta,0) = \sqrt{\frac{4\pi}{2\ell+1}}\, Y_\ell^{m'*}(\theta,\phi)$$

Eq. (3.6.52), p. 206.

$$\mathcal{D}^{(\ell)}_{m0}(\alpha,\beta,\gamma=0) = \sqrt{\frac{4\pi}{2\ell+1}}\, Y_\ell^{m*}(\beta,\alpha)$$

$$\ell=1 \quad \downarrow \alpha=0 \qquad\qquad \downarrow \alpha=0$$

$$d^{(1)}_{m0}(\beta) = \sqrt{\frac{4\pi}{3}}\, Y_1^{m*}(\beta,0)$$

$$d^{(1)}(\beta)|1,0\rangle = \sum_{m=-1,0,+1} |\ell=1,m\rangle \underbrace{\langle \ell=1,m| d^{(1)}(\beta)|1,0\rangle}_{d^{(1)}_{m0}(\beta)}$$

$$= \sqrt{\frac{4\pi}{3}} \sum_{m=-1,0,+1} Y_1^{m*}(\beta,0)\,|1,m\rangle.$$ as mentioned earlier.

Exercise : Rotation of physical space vs. Hilbert space

As $\quad R_y(\beta)\,|\theta,0\rangle = |\theta+\beta,0\rangle,$

$$\langle\theta,0|\,R_y(\beta) = \langle\theta-\beta,0|.$$

Now, consider $\quad \langle\theta,0|\,R_y(\beta)\,|1,m\rangle$

Then, this matrix element can be thought either physical space rotation as

$$\langle\theta-\beta,0|1,m\rangle$$ or Hilbert space rotation

as

$$\langle\theta,0|\sum_{m'}|1,m'\rangle\underbrace{\langle 1,m'|\,e^{-\frac{iJ_y\beta}{\hbar}}\,|1,m\rangle}_{d^{(1)}_{m'm}(\beta)}$$

$$= \sum_{m'}\langle\theta,0|1m'\rangle\,d^{(1)}_{m'm}(\beta).$$

The two must be same, i.e.

$$\langle\theta-\beta,0|1,m\rangle = \sum_{m'}\langle\theta,0|1m'\rangle\,d^{(1)}_{m'm}(\beta)$$

or $$Y_1^m(\theta-\beta,0) = \sum_{m'}Y_1^{m'}(\theta,0)\,d_{m'm}(\beta)$$

e.g. $\underline{m=0 \text{ case}}$

$$Y_1^0(\theta-\beta,0) = Y_1^1(\theta,0)\,d^{(1)}_{10}(\beta) + Y_1^0(\theta,0)\,d^{(1)}_{00}(\beta) + Y_1^{-1}(\theta,0)\,d^{(1)}_{-10}(\beta)$$

$$\sqrt{\frac{3}{4\pi}}\cos(\theta-\beta) = \left(-\sqrt{\frac{3}{8\pi}}\sin\theta\right)\left(-\frac{\sin\beta}{\sqrt{2}}\right) + \left(\sqrt{\frac{3}{4\pi}}\cos\theta\right)\cos\beta + \left(\sqrt{\frac{3}{8\pi}}\sin\theta\right)\left(\frac{\sin\beta}{\sqrt{2}}\right)$$

$$= \sqrt{\frac{3}{4\pi}}\,\big(\underbrace{\cos\theta\cos\beta + \sin\theta\sin\beta}_{\cos(\theta-\beta)}\big)$$

as it must be.

Eqs. of Spherical Harmonics

$$L_z |l,m\rangle = m\hbar |l,m\rangle$$

$$\langle\theta,\phi| L_z = \frac{\hbar}{i}\frac{\partial}{\partial\phi}\langle\theta,\phi| \qquad \left(\text{cf. } \langle x|p = \frac{\hbar}{i}\frac{\partial}{\partial x}\langle x|\right)$$

$$\boxed{\frac{\hbar}{i}\frac{\partial}{\partial\phi} Y_l^m(\theta,\phi) = m\hbar\, Y_l^m(\theta,\phi)} \rightarrow Y_l^m \sim e^{im\phi}$$

Eq. (B.5.6)

$$x = r\sin\theta\cos\phi \qquad \frac{\partial}{\partial x} = \sin\theta\cos\phi\frac{\partial}{\partial r} + \cos\theta\cos\phi\,\frac{1}{r}\frac{\partial}{\partial\theta} - \frac{\sin\phi}{r\sin\theta}\frac{\partial}{\partial\phi}$$

$$y = r\sin\theta\sin\phi \qquad \frac{\partial}{\partial y} = \sin\theta\sin\phi\frac{\partial}{\partial r} + \cos\theta\sin\phi\,\frac{1}{r}\frac{\partial}{\partial\theta} + \frac{\cos\phi}{r\sin\theta}\frac{\partial}{\partial\phi}$$

$$z = r\cos\theta \qquad \frac{\partial}{\partial z} = \cos\theta\frac{\partial}{\partial r} - \sin\theta\frac{1}{r}\frac{\partial}{\partial\theta}.$$

e.g. $x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x} = \frac{\partial}{\partial\phi}$

$$\langle\theta,\phi| L_x |l,m\rangle = \frac{\hbar}{i}\left(-\sin\phi\frac{\partial}{\partial\theta} - \cot\theta\cos\phi\frac{\partial}{\partial\phi}\right)\langle\theta,\phi|l,m\rangle$$

$$L_x \leftarrow \frac{\hbar}{i}\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)$$

$$\langle\theta,\phi| L_y |l,m\rangle = \frac{\hbar}{i}\left(\cos\phi\frac{\partial}{\partial\theta} - \cot\theta\sin\phi\frac{\partial}{\partial\phi}\right)\langle\theta,\phi|l,m\rangle$$

$$\langle\theta,\phi| \underset{L_x + iL_y}{L_+} |l,m\rangle = \frac{\hbar}{i}e^{i\phi}\left(i\frac{\partial}{\partial\theta} - \cot\theta\frac{\partial}{\partial\phi}\right)\langle\theta,\phi|l,m\rangle$$

$$= \sqrt{l(l+1) - m(m+1)}\,\hbar\,\langle\theta,\phi|l,m+1\rangle$$

Similarly, $\langle\theta,\phi| L_- |l,m\rangle = \frac{\hbar}{i}e^{-i\phi}\left(-i\frac{\partial}{\partial\theta} - \cot\theta\frac{\partial}{\partial\phi}\right)\langle\theta,\phi|l,m\rangle = \sqrt{l(l+1) - m(m-1)}\,\hbar\,\langle\theta,\phi|l,m-1\rangle$

$$\langle\theta,\phi|\vec{L}^2|l,m\rangle = \langle\theta,\phi|\ L_z^2+\frac{1}{2}(L_+L_-+L_-L_+)|l,m\rangle$$

$$= -\hbar^2\left[\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}+\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)\right]\langle\theta,\phi|l,m\rangle$$

$$= l(l+1)\hbar^2\langle\theta,\phi|l,m\rangle.$$

$$\boxed{\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}+l(l+1)\right]Y_l^m(\theta,\phi)=0}$$

Eq. (B.5.4)

To find the solutions, we may use the ladder operator technique just like what we did in SHO problem.

From $\langle\theta,\phi|L_+|l,l\rangle=0$, we get

$$\frac{\hbar}{i}e^{i\phi}\left(i\frac{\partial}{\partial\theta}-\cot\theta\frac{\partial}{\partial\phi}\right)Y_l^l(\theta,\phi)=0.$$

As $i\frac{\partial}{\partial\theta}\sin^l\theta = il\cot\theta\sin^l\theta$ and $\frac{\partial}{\partial\phi}e^{il\phi}=ile^{il\phi}$,

we get $Y_l^l(\theta,\phi)=C_l e^{il\phi}\sin^l\theta$.

Using the normalization condition $\langle l',m'|l,m\rangle=\delta_{ll'}\delta_{mm'}$, we find $\int_0^{2\pi}d\phi\int_{-1}^{+1}d\cos\theta\,|C_l|^2\sin^{2l}\theta=1$

and $C_l=\frac{(-1)^l}{2^l l!}\sqrt{\frac{(2l+1)(2l)!}{4\pi}}$, where the phase factor is inserted to get $Y_0^0=\frac{1}{\sqrt{4\pi}}$ with the phase of $P_l(\cos\theta)$ fixed by $P_l(1)=1$.

Using the recursion relation

$$Y_l^{m-1}(\theta,\phi) = \langle \theta,\phi | l, m-1 \rangle$$

$$= \frac{\langle \theta,\phi | L_- | l, m\rangle}{\sqrt{l(l+1) - m(m-1)}\,\hbar}$$

$$= \frac{1}{\sqrt{\underbrace{l(l+1)-m(m-1)}_{(l+m)(l-m+1)}}}\, e^{-i\phi}\left(-\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\phi}\right) Y_l^m(\theta,\phi)$$

we get the solutions for $m \geq 0$, i.e. $m = l, l-1, \cdots, 0$, as

$$Y_l^m(\theta,\phi) = \frac{(-1)^l}{2^l l!}\sqrt{\frac{(2l+1)(l+m)!}{4\pi\,(l-m)!}}\, e^{im\phi}$$

$$\times \frac{1}{\sin^m\theta}\frac{d^{l-m}}{d(\cos\theta)^{l-m}}(\sin^2\theta)^l ,$$

In particular,

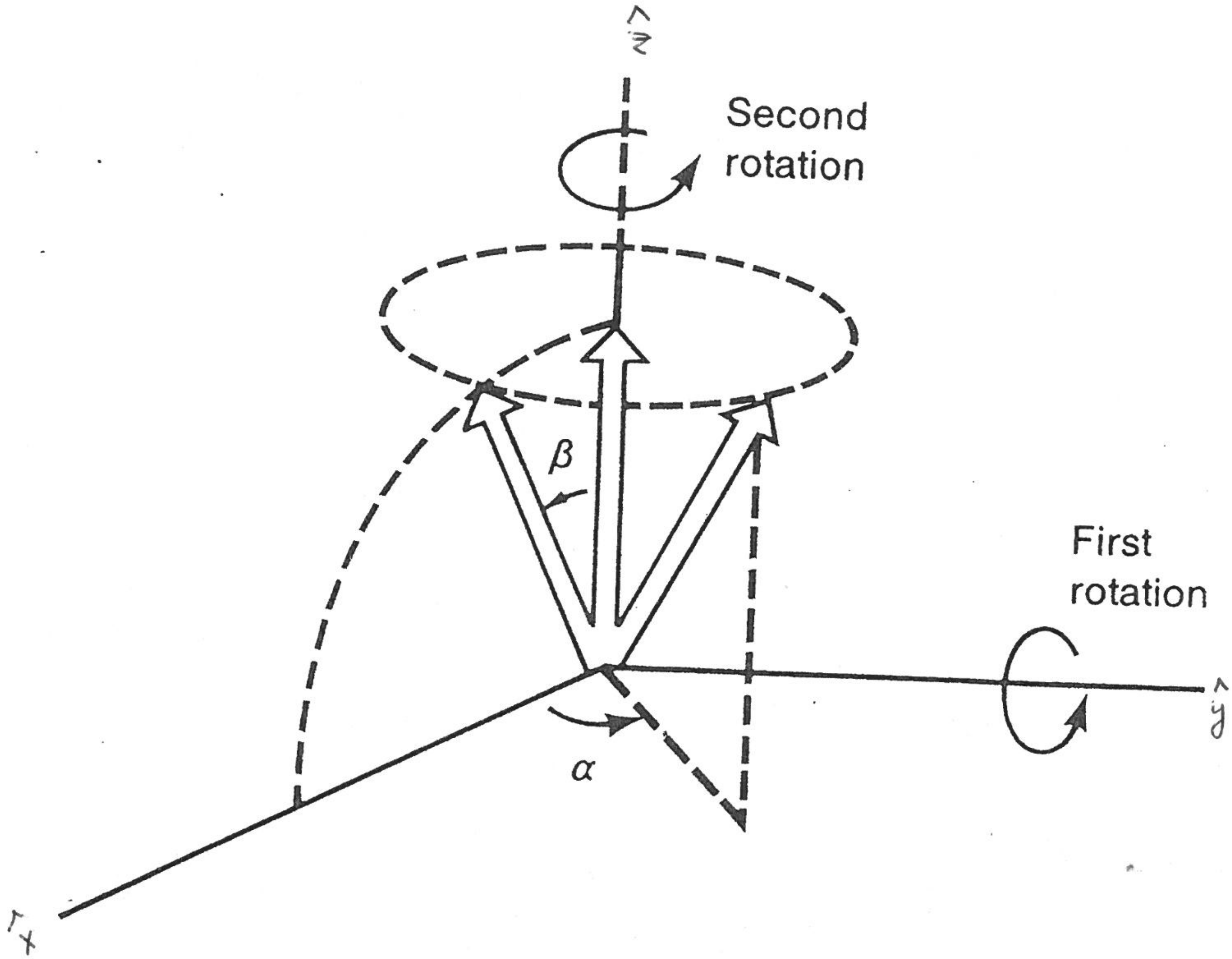
$$Y_l^0(\theta,\phi) = \frac{(-1)^l}{2^l l!}\sqrt{\frac{2l+1}{4\pi}}\frac{d^l}{d(\cos\theta)^l}(\sin^2\theta)^l$$

$$= \sqrt{\frac{2l+1}{4\pi}}\, P_l(\cos\theta),$$

where

$$P_l(\cos\theta) = \frac{(-1)^l}{2^l l!}\frac{d^l(\sin^2\theta)^l}{d(\cos\theta)^l}.$$

For $m = -1, -2, \cdots, -l$ (or $m < 0$),
one can get from $Y_l^{-m}(\theta,\phi) = (-1)^m [Y_l^m(\theta,\phi)]^*$,
where $(-1)^m$ is introduced to be consistent with $P_l^{-m} = (-1)^m\frac{(l-m)!}{(l+m)!}P_l^m$.
(Condon-Shortley's convention: $(-1)^m$ to $m \geq 0$)



$\hat{z}$
Second
rotation
β
First
rotation
$\hat{y}$
α
$\hat{x}$

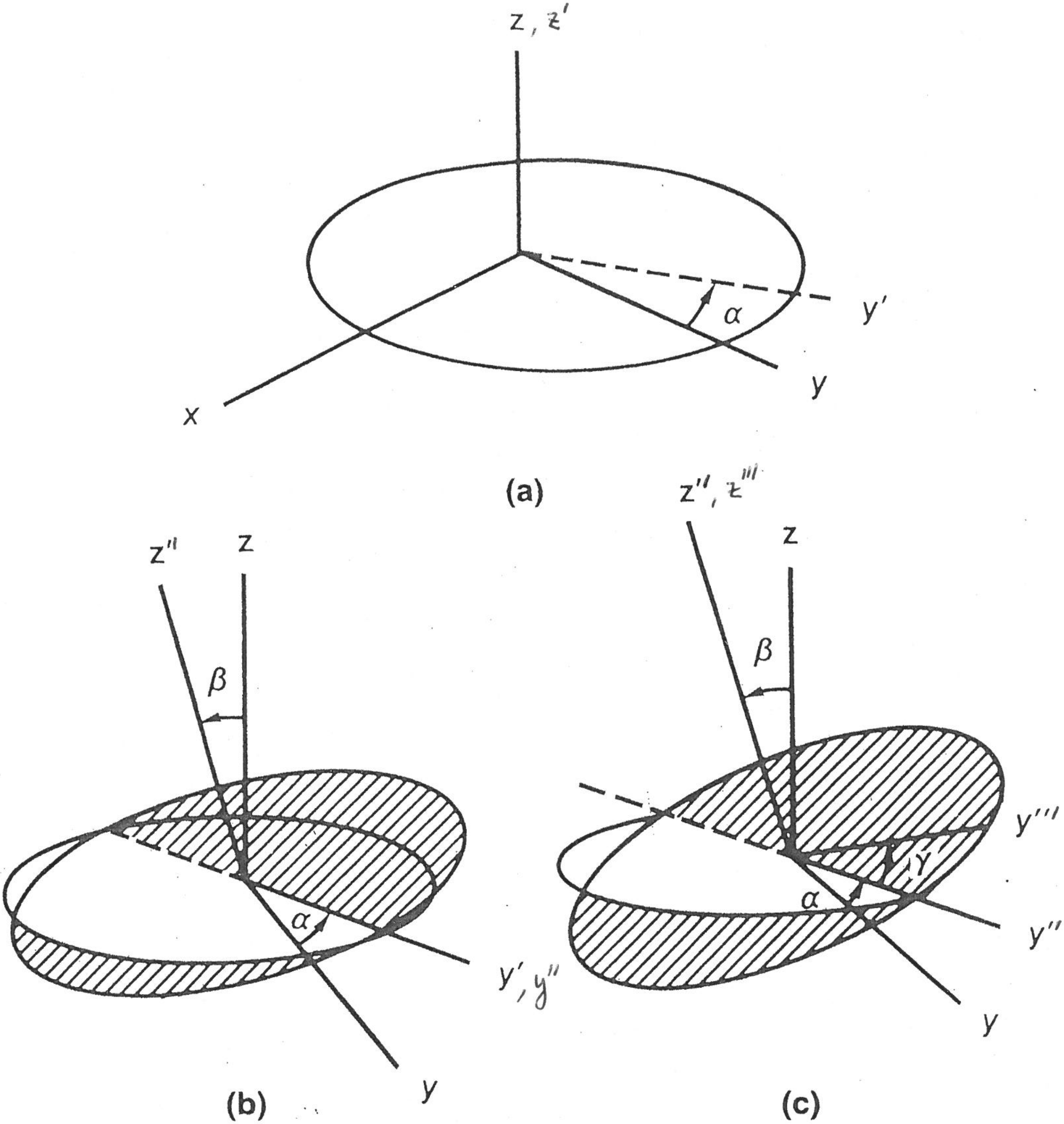


FIGURE 3.4. Euler rotations.