

Addition theorem for spherical harmonics
Masatsugu Sei Suzuki, Department of Physics
SUNY at Binghamton
(Date: January 25, 2016)

Let

$$|\mathbf{n}_1\rangle = \hat{R}(\theta_1, \phi_1)|\mathbf{e}_z\rangle = |\mathfrak{R}(\theta_1, \phi_1)\mathbf{e}_z\rangle$$

with the geometrical rotation defined by

$$\begin{aligned}\mathfrak{R}(\theta_1, \phi_1) &= \mathfrak{R}_z(\phi_1)\mathfrak{R}_y(\theta_1) = \begin{pmatrix} \cos\theta_1 \cos\phi_1 & -\sin\phi_1 & \sin\theta_1 \cos\phi_1 \\ \cos\theta_1 \sin\phi_1 & \cos\phi_1 & \sin\theta_1 \sin\phi_1 \\ -\sin\theta_1 & 0 & \cos\theta_1 \end{pmatrix} \\ \mathfrak{R}_z(\phi_1) &= \begin{pmatrix} \cos\phi_1 & -\sin\phi_1 & 0 \\ \sin\phi_1 & \cos\phi_1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \mathfrak{R}_y(\theta_1) = \begin{pmatrix} \cos\theta & 0 & \sin\theta \\ 0 & 1 & 0 \\ -\sin\theta & 0 & \cos\theta \end{pmatrix}\end{aligned}$$

The unit vector \mathbf{n}_1 is defined by

$$\begin{aligned}\mathbf{n}_1 &= \mathfrak{R}(\theta_1, \phi_1)\mathbf{e}_z \\ &= \begin{pmatrix} \cos\theta_1 \cos\phi_1 & -\sin\phi_1 & \sin\theta_1 \cos\phi_1 \\ \cos\theta_1 \sin\phi_1 & \cos\phi_1 & \sin\theta_1 \sin\phi_1 \\ -\sin\theta_1 & 0 & \cos\theta_1 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \\ &= \begin{pmatrix} \sin\theta_1 \cos\phi_1 \\ \sin\theta_1 \sin\phi_1 \\ \cos\theta_1 \end{pmatrix}\end{aligned}$$

Another ket $|\mathbf{n}_2\rangle$ is defined by

$$|\mathbf{n}_2\rangle = \hat{R}(\theta_2, \phi_2)|\mathbf{e}_z\rangle = |\mathfrak{R}(\theta_2, \phi_2)\mathbf{e}_z\rangle$$

where the geometrical rotation matrix is given by

$$\mathfrak{R}(\theta_2, \phi_2) = \mathfrak{R}_z(\phi_2) \mathfrak{R}_y(\theta_2) = \begin{pmatrix} \cos \theta_2 \cos \phi_2 & -\sin \phi_2 & \sin \theta_2 \cos \phi_2 \\ \cos \theta_2 \sin \phi_2 & \cos \phi_2 & \sin \theta_2 \sin \phi_2 \\ -\sin \theta_2 & 0 & \cos \theta_2 \end{pmatrix}$$

Note that

$$\begin{aligned} \mathbf{n}_2 &= \mathfrak{R}(\theta_2, \phi_2) \mathbf{e}_z \\ &= \begin{pmatrix} \cos \theta_2 \cos \phi_2 & -\sin \phi_2 & \sin \theta_2 \cos \phi_2 \\ \cos \theta_2 \sin \phi_2 & \cos \phi_2 & \sin \theta_2 \sin \phi_2 \\ -\sin \theta_2 & 0 & \cos \theta_2 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \\ &= \begin{pmatrix} \sin \theta_2 \cos \phi_2 \\ \sin \theta_2 \sin \phi_2 \\ \cos \theta_2 \end{pmatrix} \end{aligned}$$

Then we have the inner product as

$$\mathbf{n}_1 \cdot \mathbf{n}_2 = \cos \theta_1 \cos \theta_2 + \sin \theta_1 \sin \theta_2 \cos(\phi_1 - \phi_2)$$

We assume a new ket defined by

$$|\mathbf{n}'\rangle = \hat{R}^{-1}(\theta_1, \phi_1) |\mathbf{n}_2\rangle = |\mathfrak{R}^{-1}(\theta_1, \phi_1) \mathbf{n}_2\rangle,$$

and

$$\langle \mathbf{n}' | = \langle \mathbf{n}_2 | \hat{R}(\theta_1, \phi_1)$$

Note that the matrix $\mathfrak{R}^{-1}(\theta_1, \phi_1)$ is given by

$$\mathfrak{R}^{-1}(\theta_1, \phi_1) = \begin{pmatrix} \cos \theta_1 \cos \phi_1 & \cos \theta_1 \sin \phi_1 & -\sin \theta_1 \\ -\sin \phi_1 & \cos \phi_1 & 0 \\ \sin \theta_1 \cos \phi_1 & \sin \theta_1 \sin \phi_1 & \cos \theta_1 \end{pmatrix}$$

and

$$\begin{aligned}
\mathbf{n}' &= \mathfrak{R}^{-1}(\theta_1, \phi_1) \mathbf{n}_2 \\
&= \begin{pmatrix} -\sin \theta_1 \cos \theta_2 + \cos \theta_1 \sin \theta_2 \cos(\phi_1 - \phi_2) \\ -\sin \theta_2 \sin(\phi_1 - \phi_2) \\ \cos \theta_1 \cos \theta_2 + \sin \theta_1 \sin \theta_2 \cos(\phi_1 - \phi_2) \end{pmatrix} \\
&= \mathfrak{R}(\Theta, \Phi) \mathbf{e}_z \\
&= \begin{pmatrix} \sin \Theta \cos \Phi \\ \sin \Theta \sin \Phi \\ \cos \Theta \end{pmatrix}
\end{aligned}$$

Since

$$\mathbf{n}' \cdot \mathbf{e}_z = \cos \theta_1 \cos \theta_2 + \sin \theta_1 \sin \theta_2 \cos(\phi_1 - \phi_2)$$

it is found that

$$\mathbf{n}_1 \cdot \mathbf{n}_2 = \mathbf{n}' \cdot \mathbf{e}_z = \cos \Theta$$

In other words, Θ is the angle between \mathbf{n}' and \mathbf{e}_z and it is also the angle between \mathbf{n}_1 and \mathbf{n}_2 .

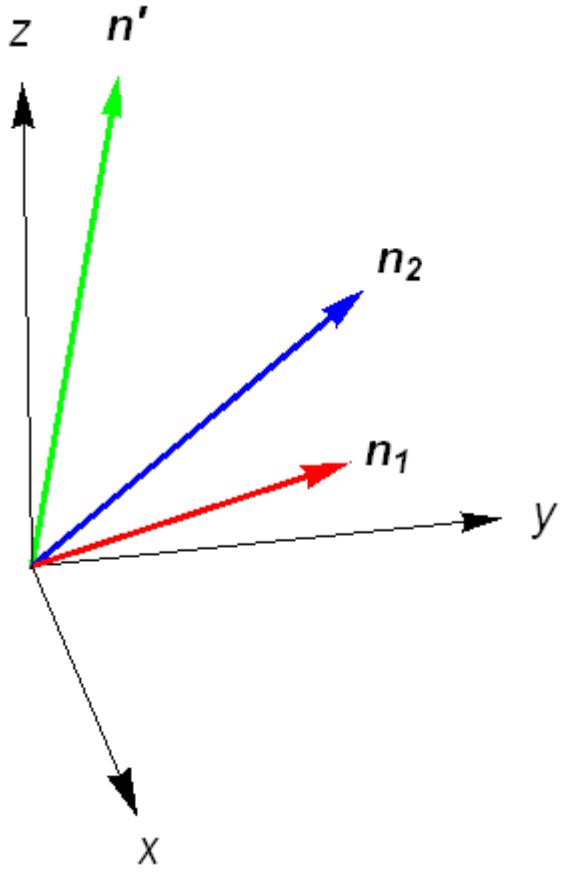


Fig. Three vectors $\mathbf{n}_1 = \Re(\theta_1, \phi_1) \mathbf{e}_z$, $\mathbf{n}_2 = \Re(\theta_2, \phi_2) \mathbf{e}_z$, $\mathbf{n}' = \Re^{-1}(\theta_1, \phi_1) \mathbf{n}_2 = \Re(\Theta, \Phi) \mathbf{e}_z$. The Mathematica is used for this figure. $\theta_1 = 60^\circ$, $\theta_2 = 45^\circ$, $\phi_1 = 30^\circ$, $\phi_2 = 50^\circ$. Without Mathematica, it is hard for me to get the line for the unit vector \mathbf{n}' .

Using the closure relation, we get

$$\begin{aligned}
 Y_l^m(\Theta, \Phi) &= \langle \mathbf{n}' | l, m \rangle \\
 &= \langle \mathbf{n}_2 | \hat{R}(\theta_1, \phi_1) | l, m \rangle \\
 &= \sum_{m'} \langle \mathbf{n}_2 | l, m' \rangle \langle l, m' | \hat{R}(\theta_1, \phi_1) | l, m \rangle \\
 &= \sum_{m'} Y_l^{m'}(\theta_2, \phi_2) \langle l, m' | \hat{R}(\theta_1, \phi_1) | l, m \rangle
 \end{aligned} \tag{1}$$

where

$$D_{m'm}^{(l)}(\theta_1, \phi_1) = \langle l, m' | \hat{R}(\theta_1, \phi_1) | l, m \rangle$$

Equation (1) relates spherical harmonics in three different directions. The most useful case is $m = 0$;

$$D_{m'm=0}^{(l)}(\theta_1, \phi_1) = e^{-im'\phi_1} d_{m'm=0}^{(l)}(\theta_1)$$

where

$$d_{m'm=0}^{(l)}(\theta_1) = e^{im'\phi_1} \sqrt{\frac{4\pi}{2l+1}} [Y_l^{m'}(\theta_1, \phi_1)]^*$$

and

$$d_{m'=0, m=0}^{(l)}(\theta_1) = \sqrt{\frac{4\pi}{2l+1}} [Y_l^{m'=0}(\theta_1, \phi_1)]^* = P_l(\cos \theta_1)$$

Then we have

$$\begin{aligned} Y_l^{m=0}(\Theta, \Phi) &= \sum_{m'} Y_l^{m'}(\theta_2, \phi_2) D_{m'm=0}^{(l)}(\theta_1, \phi_1) \\ &= \sum_{m'} Y_l^{m'}(\theta_2, \phi_2) e^{-im'\phi_1} d_{m'm=0}^{(l)}(\theta_1) \\ &= \sqrt{\frac{4\pi}{2l+1}} \sum_{m'} e^{-im'\phi_1} e^{im'\phi_1} [Y_l^{m'}(\theta_1, \phi_1)]^* Y_l^{m'}(\theta_2, \phi_2) \\ &= \sqrt{\frac{4\pi}{2l+1}} \sum_m [Y_l^m(\theta_1, \phi_1)]^* Y_l^m(\theta_2, \phi_2) \end{aligned}$$

which leads to the addition theorem for the spherical harmonics

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

(a)

$$|\mathbf{n}'\rangle = \hat{R} |\mathbf{n}\rangle, \quad |\mathbf{n}\rangle = \hat{R}^+ |\mathbf{n}'\rangle, \quad \langle \mathbf{n}| = \langle \mathbf{n}'| \hat{R}$$

Using the closure relation, we get

$$\hat{R}|l,m\rangle = \sum_{m'} |l,m'\rangle \langle l,m'|\hat{R}|l,m\rangle$$

and

$$\langle \mathbf{n}'|\hat{R}|l,m\rangle = \sum_{m'} \langle \mathbf{n}'|l,m'\rangle \langle l,m'|\hat{R}|l,m\rangle$$

Noting that $\langle \mathbf{n}| = \langle \mathbf{n}'|\hat{R}$, we get

$$\langle \mathbf{n}|l,m\rangle = \sum_{m'} \langle \mathbf{n}'|l,m'\rangle \langle l,m'|\hat{R}|l,m\rangle$$

or

$$Y_l^m(\mathbf{n}) = \sum_{m'} Y_l^{m'}(\mathbf{n}') D_{m',m}^{(l)}(\hat{R})$$

(b)

$$|\mathbf{n}\rangle = \hat{R}|\mathbf{n}'\rangle, \quad \langle \mathbf{n}| = \langle \mathbf{n}'|\hat{R}^+$$

Using the closure relation, we get

$$\hat{R}^+|l,m\rangle = \sum_{m'} |l,m'\rangle \langle l,m'|\hat{R}^+|l,m\rangle$$

and

$$\langle \mathbf{n}'|\hat{R}^+|l,m\rangle = \sum_{m'} \langle \mathbf{n}'|l,m'\rangle \langle l,m'|\hat{R}^+|l,m\rangle$$

Noting that $\langle \mathbf{n}| = \langle \mathbf{n}'|\hat{R}^+$, we get

$$\langle \mathbf{n}|l,m\rangle = \sum_{m'} \langle \mathbf{n}'|l,m'\rangle \langle l,m'|\hat{R}^+|l,m\rangle$$

or

$$Y_l^m(\pmb{n})=\sum_{m'}Y_l^{m'}(\pmb{n}')D_{m',m}^{(l)}(\hat{R})$$