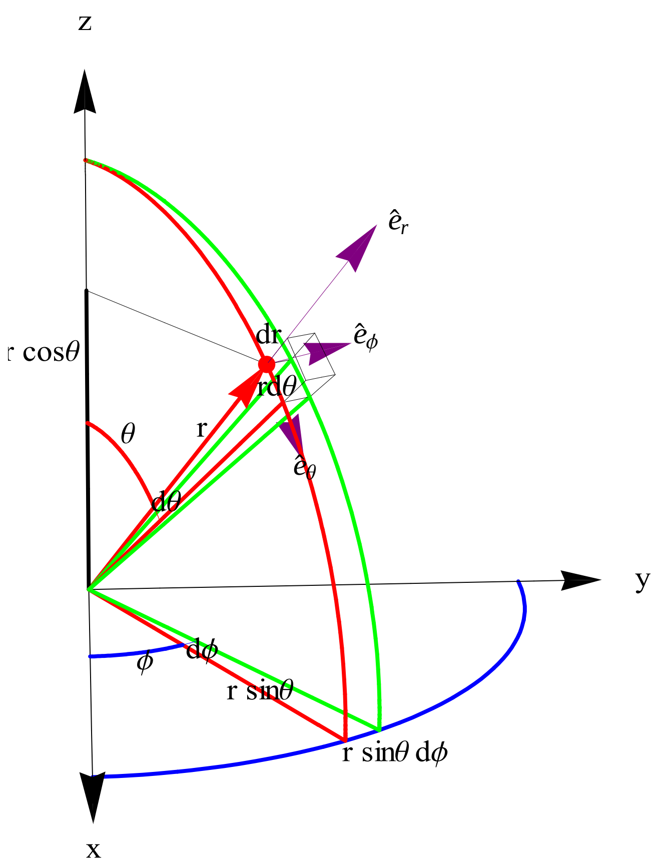
**Chapter 23**
**Spherical Harmonics**
**Masatsugu Suzuki**
**Department of Physics, SUNY at Binghamton**
**(Date: November 22, 2010)**

Spherical harmonics
Dirac delta function
Addition theorem
Recurrence relation
Associated Legendre functions
Parity
SphericalPlot3D

## 23.1 Formulation




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

$$\hat{L}_z|l,m\rangle = m\hbar|l,m\rangle$$

or

$$\langle \mathbf{n}|\hat{L}_z|l,m\rangle = -i\hbar\frac{\partial}{\partial\phi}\langle \mathbf{n}|l,m\rangle = m\hbar\langle \mathbf{n}|l,m\rangle$$

$$|\mathbf{n}\rangle = |\theta,\phi\rangle$$

The closure relation

$$\int|\theta,\phi\rangle d\Omega\langle\theta,\phi| = \hat{1}$$

where

$$d\Omega = \sin\theta d\theta d\phi$$

The $\theta$ and $\phi$ dependence of $\langle \mathbf{n}|l,m\rangle$ is given by

$$\begin{aligned}\langle \mathbf{n}|\hat{L}^2|lm\rangle &= -\hbar^2[\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2} + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\frac{\partial}{\partial\theta})]Y_l^m(\theta,\phi) \\ &= \hbar^2 l(l+1)Y_l^m(\theta,\phi)\end{aligned} \tag{1}$$

$$\langle \mathbf{n}|\hat{L}_z|lm\rangle = \frac{\hbar}{i}\frac{\partial}{\partial\phi}Y_l^m(\theta,\phi) = \hbar m Y_l^m(\theta,\phi) \tag{2}$$

Equation (2) shows that

$$Y_l^m(\theta,\phi) = \Theta_l^m(\theta)e^{im\phi}$$

We must require that the eigenfunction be single valued

$$e^{im\phi} = e^{im(\phi+2\pi)}$$

which means that $m = 0, \pm 1, \pm 2,$ (integers). Equation (1) can be rewritten as

$$[\frac{1}{\sin\theta}\frac{d}{d\theta}(\sin\theta\frac{d}{d\theta}) - \frac{m^2}{\sin^2\theta} + l(l+1)]\Theta_l^m(\theta) = 0$$

The orhogonality relation $\langle l',m'|l,m\rangle = \delta_{l,l'}\delta_{m,m'}$ leads to

$$\delta_{l,l'}\delta_{m,m'} = \int d\Omega\langle l',m'|\mathbf{n}\rangle\langle\mathbf{n}|l,m\rangle = \iint \sin\theta d\theta d\phi Y_{l'}^{m'^*}(\theta,\phi)Y_l^m(\theta,\phi)$$

To obtain the form of $Y_l^m(\theta,\phi)$, we may start with $m = l$.

$$\hat{L}_+|l,m=l\rangle = 0$$

or

$$\langle\mathbf{n}|\hat{L}_+|l,m=l\rangle = -i\hbar e^{i\phi}(i\frac{\partial}{\partial\theta} - \cot\theta\frac{\partial}{\partial\phi})\langle\mathbf{n}|l,m=l\rangle = 0$$

Since $\langle\mathbf{n}|l,m=l\rangle = Y_l^l(\theta,\phi) = \Theta_l^l(\theta)e^{il\phi}$

$$(\frac{d}{d\theta} - l\cot\theta)\Theta_l^l(\theta) = 0$$

or

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

where $C_l$ is a normalization constant.

$$C_l = \frac{(-1)^l}{2^l l!}\sqrt{\frac{(2l+1)(2l)!}{4\pi}}$$

The result for $m \geq 0$ is

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

and we define $Y_l^{-m}(\theta,\phi)$ by

$$Y_l^{-m}(\theta,\phi) = (-1)^m[Y_l^m(\theta,\phi)]^*$$

or

$$[Y_l^m(\theta,\phi)]^* = (-1)^m Y_l^{-m}(\theta,\phi)$$

## 23.2 Dirac delta function

The Dirac delta function can be described by

$$\delta(\mathbf{r}-\mathbf{r}')=\frac{1}{r^2}\delta(r-r')\delta(\mathbf{n}-\mathbf{n}')$$

since

$$\int d^3\mathbf{r}'\delta(\mathbf{r}-\mathbf{r}')=\int\frac{1}{r'^2}\delta(r-r')r'^2dr'\int d\Omega'\delta(\mathbf{n}-\mathbf{n}')=\int d\Omega'\delta(\mathbf{n}-\mathbf{n}')=1$$

Here we note that

$$\begin{aligned}\langle\mathbf{n}|\mathbf{n}'\rangle=\delta(\mathbf{n}-\mathbf{n}')&=\sum_{l=0}^{\infty}\sum_{m=-l}^{l}\langle\mathbf{n}|l,m\rangle\langle l,m|\mathbf{n}'\rangle\\&=\sum_{l=0}^{\infty}\sum_{m=-l}^{l}Y_l^{m^*}(\theta',\phi')Y_l^m(\theta,\phi)\qquad,\\&=\sum_{l=0}^{\infty}\frac{2l+1}{4\pi}P_l(\mathbf{n}\cdot\mathbf{n}')\end{aligned}$$

where we use the addition theorem (see Chapter 19)

$$P_l(\mathbf{n}\cdot\mathbf{n}')=\frac{4\pi}{2l+1}\sum_{m=-l}^{l}Y_l^m(\theta,\phi)Y_l^{m^*}(\theta',\phi')$$

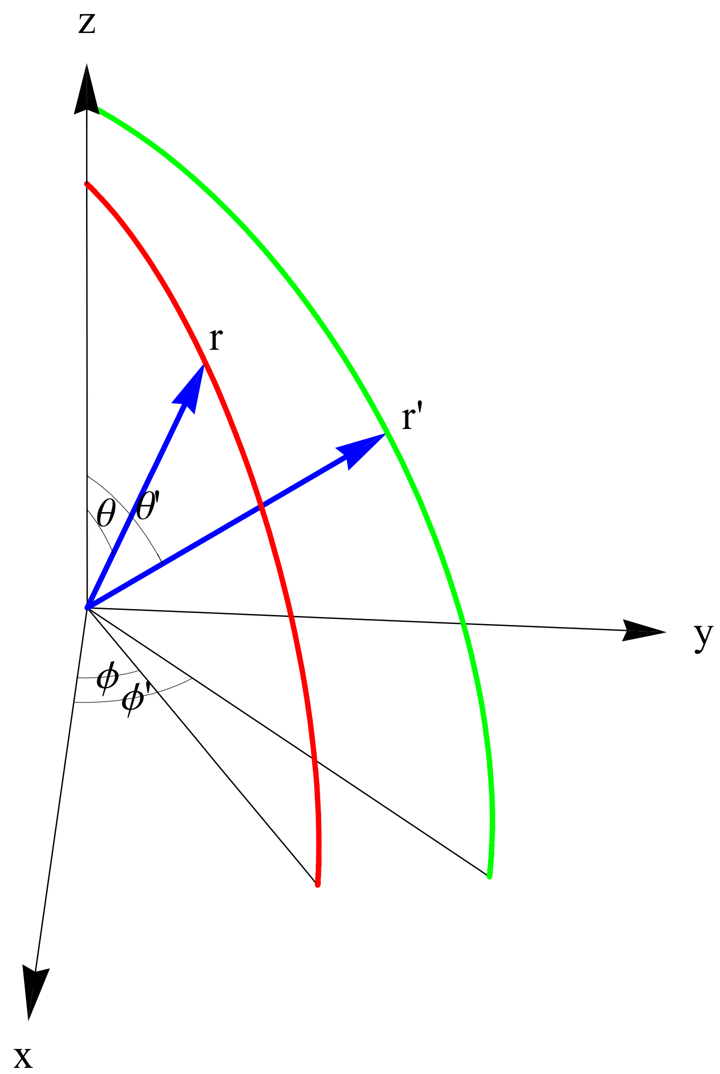



Fig. Angle $\gamma$ such that $\mathbf{n}\cdot\mathbf{n}' = \dfrac{\mathbf{r}\cdot\mathbf{r}'}{rr'} = \cos\gamma$

In summary, the Dirac delta function is expressed by

$$\boxed{\begin{aligned}\delta(\mathbf{r}-\mathbf{r}') &= \frac{1}{r^2}\delta(r-r')\delta(\mathbf{n}-\mathbf{n}') \\ &= \frac{1}{r^2}\delta(r-r')\sum_{l=0}^{\infty}\frac{2l+1}{4\pi}P_l(\mathbf{n}\cdot\mathbf{n}')\end{aligned}}$$

This formula will be useful in the theory of scattering from a spherical potential.

## 23.3 Associate Legendre function

$Y_l^m(\theta,\phi)$ can be also expressed by

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

where $P_l^m(\cos\theta)$ is the associated Legendre function.

$$\begin{aligned} P_l^m(x) &= (1-x^2)^{m/2}\frac{d^m}{dx^m}P_l(x) \\ &= \frac{1}{2^l l!}(1-x^2)^{m/2}\frac{d^{l+m}}{dx^{l+m}}(x^2-1)^l \end{aligned} \qquad \text{for } m \geq 0.$$

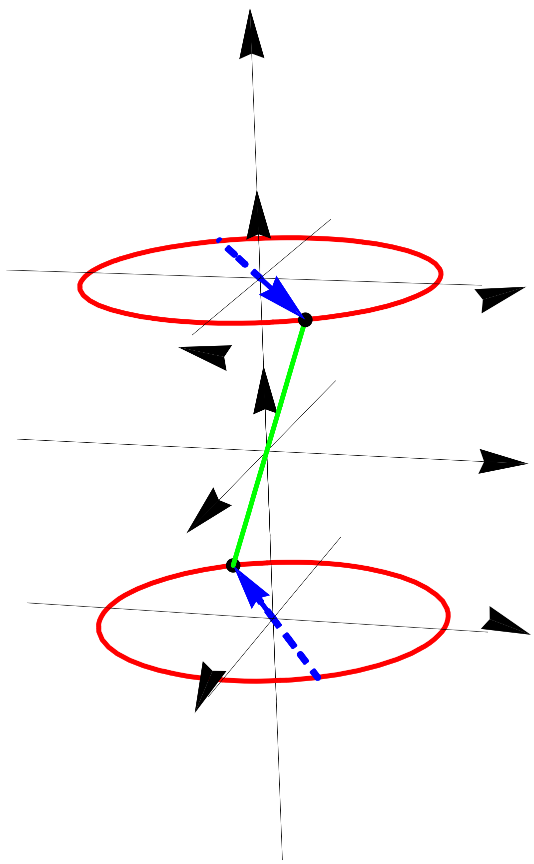
$$P_l^{-m}(x) = (-1)^m \frac{(l-m)!}{(l+m)!} P_l^m(x)$$

$$P_l^0(x) = P_l(x) = \frac{1}{2^l l!}\frac{d^l}{dx^l}(x^2-1)^l$$

$$P_l(1) = 1$$

$$P_l(-1) = (-1)^l$$

## 23.4 Parity



$$\hat{\pi}|\mathbf{n}\rangle = |-\mathbf{n}\rangle, \text{ or } \langle\mathbf{n}|\hat{\pi} = \langle-\mathbf{n}|$$

For ***n*** to **-*n***, we have

$$\theta \to \pi - \theta, \text{ and } \phi \to \pi + \phi$$

$$\langle\mathbf{n}|\hat{\pi}|l,m\rangle = \langle-\mathbf{n}|l,m\rangle = Y_l^m(\pi-\theta,\pi+\phi) = (-1)^l Y_l^m(\theta,\phi) = (-1)^l\langle\mathbf{n}|l,m\rangle$$

or

$$\hat{\pi}|l,m\rangle = (-1)^l|l,m\rangle$$

Note that

$$\hat{\pi}\hat{L}_{\pm}\hat{\pi} = \hat{L}_{\pm}, \qquad \text{or} \qquad \hat{\pi}\hat{L}_{\pm} = \hat{L}_{\pm}\hat{\pi}$$

$$\hat{\pi}\hat{L}_{\pm}|l,0\rangle = \hat{L}_{\pm}\hat{\pi}|l,0\rangle$$

Here we suppose that $|l,0\rangle$ is the state with either even or odd parity

$$\hat{\pi}|l,0\rangle = p_e|l,0\rangle$$

Then we have

$$\hat{\pi}\hat{L}_{\pm}|l,0\rangle = \hat{L}_{\pm}\hat{\pi}|l,0\rangle = p_e\hat{L}_{\pm}|l,0\rangle$$

This implies that $\hat{L}_{\pm}|l,0\rangle$ has also the same parity as the state $|l,0\rangle$. Repeating this procedure, we can find that the parity of the state $|l,m\rangle$ is the same as that of the state $|l,0\rangle$. The problem is reduced to the determination of the parity of the state $|l,0\rangle$.

$$\langle\mathbf{n}|\hat{\pi}|l,0\rangle = \langle-\mathbf{n}|l,0\rangle = p_e\langle\mathbf{n}|l,0\rangle$$

Here

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

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

when $\theta \to \pi - \theta$.

Therefore we have

$$\hat{\pi}|l,m\rangle = (-1)^l|l,m\rangle$$

## 23.5 Recurrence relation (Mathematica)

For $m = 0$,

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

which can be written in the form

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

where

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

or

$$P_l(x) = \frac{(-1)^l}{2^l l!} \frac{d^l}{dx^l} (1-x^2)^l$$

$P_l(x)$ is the $l$-th order Legendre polynomial. It has $l$ zeros in the interval $-1 \le x \le 1$. Note that $P_l(1)=1$.

$$P_l(-x) = (-1)^l P_l(x)$$

(i) $\hat{L}_-$

Through the repeat action of $\hat{L}_-$, we construct

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

with $m = l$, $l$-1, $l$-2,.....,

$$\begin{aligned}
\langle \mathbf{n} | l,m-1 \rangle &= \frac{\langle \mathbf{n} | \hat{L}_- | l,m \rangle}{\sqrt{(l+m)(l-m+1)}\hbar} \\
&= \frac{1}{\sqrt{(l+m)(l-m+1)}\hbar} (-i\hbar e^{-i\phi})(-i\frac{\partial}{\partial\theta} - \cot\theta \frac{\partial}{\partial\phi}) \langle \mathbf{n} | l,m \rangle \\
&= \frac{1}{\sqrt{(l+m)(l-m+1)}} e^{-i\phi} (-\frac{\partial}{\partial\theta} + i\cot\theta \frac{\partial}{\partial\phi}) \langle \mathbf{n} | l,m \rangle
\end{aligned}$$

(recurrence relation)

(ii) $\hat{L}_+$

Through the repeat action of $\hat{L}_+$, we construct

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

with $m = 0,1, 2,....., l$:

$$\langle \mathbf{n}|l,m+1\rangle = \frac{\langle \mathbf{n}|\hat{L}_+|l,m\rangle}{\sqrt{(l-m)(l+m+1)}\hbar}$$

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

Here we use

$$\langle \mathbf{n}|l,m=0\rangle = \sqrt{\frac{2l+1}{4\pi}}P_l(\cos\theta)\,.$$

((**Mathematica**))
Using recurrence relation for spherical harmonics, we get spherical harmonics

```
Clear["Global`*"];

OG[ℓ_, m_] := 1/Sqrt[(ℓ + m) (ℓ - m + 1)] Exp[-ⅈ ϕ] (-D[#, θ] + ⅈ Cot[θ] D[#, ϕ]) &;

H[ℓ_, m_, θ_, ϕ_] := OG[ℓ, m + 1][H[ℓ, m + 1, θ, ϕ]];

H[1, 1, θ, ϕ] = SphericalHarmonicY[1, 1, θ, ϕ];
```

**l = 1, m = 1, 0, -1**

```
Table[{1, m, H[1, m, θ, ϕ], SphericalHarmonicY[1, m, θ, ϕ] },
  {m, 1, -1, -1}] // Simplify // TableForm
```

| | | | |
|---|---|---|---|
| 1 | 1 | $-\frac{1}{2} e^{i\phi}\sqrt{\frac{3}{2\pi}}$ Sin[θ] | $-\frac{1}{2} e^{i\phi}\sqrt{\frac{3}{2\pi}}$ Sin[θ] |
| 1 | 0 | $\frac{1}{2}\sqrt{\frac{3}{\pi}}$ Cos[θ] | $\frac{1}{2}\sqrt{\frac{3}{\pi}}$ Cos[θ] |
| 1 | -1 | $\frac{1}{2} e^{-i\phi}\sqrt{\frac{3}{2\pi}}$ Sin[θ] | $\frac{1}{2} e^{-i\phi}\sqrt{\frac{3}{2\pi}}$ Sin[θ] |

## 23.6 Useful formula (summary)

---

1.

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

$$\langle l,m|\mathbf{n}\rangle = \langle \mathbf{n}|l,m\rangle^* = Y_l^{m^*}(\theta,\phi)$$

---

2. Orthogonality

$$\langle l',m'|l,m\rangle = \delta_{l,l'}\delta_{m.m'} = \int d\Omega \langle l'.m'|\mathbf{n}\rangle\langle \mathbf{n}|l,m\rangle$$
$$= \int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta d\theta Y_{l'}^{m'^*}(\theta,\phi) Y_l^m(\theta,\phi)$$

where

$$d\Omega = \sin\theta d\theta d\phi$$

---

3.

$$\langle \mathbf{e}_z|l,m\rangle = Y_l^m(\theta=0,\phi) = \sqrt{\frac{2l+1}{4\pi}}\delta_{m,0}$$

---

4.

$$\langle \mathbf{n}|l,m=0\rangle = Y_l^0(\theta,\phi) = \sqrt{\frac{2l+1}{4\pi}}P_l(\cos\theta)$$

---

5.

$$|\mathbf{n}\rangle = \hat{R}|\mathbf{e}_z\rangle, \qquad \langle n| = \langle \mathbf{e}_z|\hat{R}$$

where $\hat{R} = \hat{R}_z(\phi)\hat{R}_y(\theta)$ is the rotation operator (see Chapter 27)

$$\langle l,m|\mathbf{n}\rangle = \langle \mathbf{n}|l,m\rangle^*$$
$$= [Y_\ell^m(\theta,\phi)]^*$$
$$= \langle l,m|\hat{R}|\mathbf{e}_z\rangle$$
$$= \sum_{m'}\langle l,m|\hat{R}|l,m'\rangle\langle l,m'|\mathbf{e}_z\rangle$$
$$= \sqrt{\frac{2\ell+1}{4\pi}}\sum_{m'}\langle l,m|\hat{R}|l,m'\rangle\delta_{m',0}$$
$$= \sqrt{\frac{2\ell+1}{4\pi}}\langle l,m|\hat{R}|l,0\rangle$$
$$= \sqrt{\frac{2\ell+1}{4\pi}}D_{m,0}^{(l)}(\hat{R})$$

or

$$D^{(l)}_{m,0}(\hat{R}) = \langle l,m|\hat{R}|l,0\rangle = \sqrt{\frac{4\pi}{2\ell+1}}[Y_\ell^m(\theta,\phi)]^* .$$

---

**6.**

$$\langle \mathbf{n}|\hat{R}|l,m\rangle = \langle e_z|\hat{R}^+\hat{R}|l,m\rangle = \langle \mathbf{e}_z|l,m\rangle$$

$$\begin{aligned}\langle \mathbf{n}|\hat{R}|l,m\rangle = \langle \mathbf{e}_z|l,m\rangle &= \sum_{m'=-l}^{l}\langle \mathbf{n}|l,m'\rangle\langle l,m'|\hat{R}|l,m\rangle \\ &= \sum_{m'=-l}^{l}\langle \mathbf{n}|l,m'\rangle\langle l,m'|\hat{R}|l,m\rangle \\ &= \sum_{m'=-l}^{l}\langle \mathbf{n}|l,m'\rangle D^{(l)}_{m',m}(\hat{R})\end{aligned}$$

or

$$\langle \mathbf{e}_z|l,m\rangle = \sqrt{\frac{2l+1}{4\pi}}\delta_{m,0} = \sum_{m'=-l}^{l}\langle \mathbf{n}|l,m'\rangle D^{(l)}_{m',m}(\hat{R})\,\mathbf{.}$$

We also have

$$\begin{aligned}\langle \mathbf{n}|l,m\rangle = \langle \mathbf{e}_z|\hat{R}^+|l,m\rangle &= \sum_{m'=-l}^{l}\langle \mathbf{e}_z|l,m'\rangle\langle l,m'|\hat{R}^+|l,m\rangle \\ &= \sum_{m'=-l}^{l}\langle \mathbf{e}_z|l,m'\rangle\langle l,m|\hat{R}|l,m'\rangle^* \\ &= \sum_{m'=-l}^{l}\langle \mathbf{e}_z|l,m'\rangle\langle l,m|\hat{R}|l,m'\rangle^* \\ &= \sum_{m'=-l}^{l}\langle \mathbf{e}_z|l,m'\rangle D^{(l)}_{m,m'}{}^*(\hat{R}) \\ &= \sqrt{\frac{2l+1}{4\pi}}\sum_{m'=-l}^{l}\delta_{m',0}D^{(l)}_{m,m'}{}^*(\hat{R}) \\ &= \sqrt{\frac{2l+1}{4\pi}}D^{(l)}_{m,0}{}^*(\hat{R})\end{aligned}$$

since

$$\langle \mathbf{e}_z | l,m \rangle = Y_l^m(\theta = 0, \phi) = \sqrt{\frac{2l+1}{4\pi}}\delta_{m,0}$$

In summary, we get

$$\sqrt{\frac{2l+1}{4\pi}} D_{m,0}^{(l)\,*}(\hat{R}) = \langle \mathbf{n} | l,m \rangle$$

or

$$D_{m,0}^{(l)\,*}(\hat{R}) = \sqrt{\frac{4\pi}{2l+1}} \langle \mathbf{n} | l,m \rangle = \sqrt{\frac{4\pi}{2l+1}} Y_l^m(\mathbf{n})$$

---

7.

$$\begin{aligned}
\langle \mathbf{n} | \mathbf{n}' \rangle = \delta(\mathbf{n} - \mathbf{n}') &= \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \langle \mathbf{n} | l,m \rangle \langle l,m | \mathbf{n}' \rangle \\
&= \sum_{l=0}^{\infty} \sum_{m=-l}^{l} Y_l^{m\,*}(\theta', \phi') Y_l^m(\theta, \phi) \qquad , \\
&= \sum_{l=0}^{\infty} \frac{2l+1}{4\pi} P_l(\mathbf{n} \cdot \mathbf{n}')
\end{aligned}$$

where we use the addition theorem

$$P_l(\mathbf{n} \cdot \mathbf{n}') = \frac{4\pi}{2l+1} \sum_{m=-l}^{l} Y_l^m(\theta, \phi) Y_l^{m\,*}(\theta', \phi')$$

---

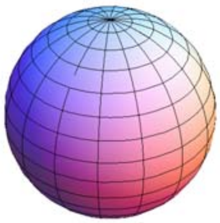
## 23.7 SphericalPlot3D of $\left| Y_l^m(\theta, \phi) \right|^2$

---

(i) $\langle n | l = 0, m = 0 >$

$l$=0 $m$=0 $Y_{l=0}^{0}(\theta, \phi)$

0 0 $\frac{1}{2\sqrt{\pi}}$

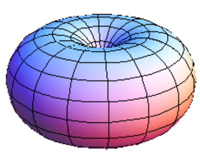


$l = 0, m = 0$

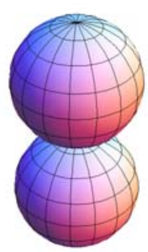
(ii) $\langle n | l = 1, m >$ ($m$ = -1, 0, 1)

$l$=1 $m$ $Y^m_{l=1}(\theta,\phi)$

| | | |
|---|---|---|
| 1 | -1 | $\frac{1}{2} e^{-i\phi} \sqrt{\frac{3}{2\pi}}$ Sin[$\theta$] |
| 1 | 0 | $\frac{1}{2} \sqrt{\frac{3}{\pi}}$ Cos[$\theta$] |
| 1 | 1 | $-\frac{1}{2} e^{i\phi} \sqrt{\frac{3}{2\pi}}$ Sin[$\theta$] |



$l = 1, m = \pm 1$



$l = 1, m = 0$

(ii) $\langle n | l = 2, m >$ ($m$ = -2, -1, 0, 1, 2)

$l$=2 $m$ $Y^m_{l=2}(\theta,\phi)$

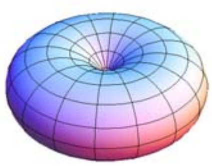
$2 \quad -2 \quad \frac{1}{4}\, e^{-2 i \phi} \sqrt{\frac{15}{2\pi}}\ \mathrm{Sin}[\theta]^2$

$2 \quad -1 \quad \frac{1}{2}\, e^{-i \phi} \sqrt{\frac{15}{2\pi}}\ \mathrm{Cos}[\theta]\ \mathrm{Sin}[\theta]$

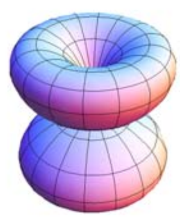
$2 \quad 0 \quad \frac{1}{8} \sqrt{\frac{5}{\pi}}\ (1 + 3\, \mathrm{Cos}[2\theta])$

$2 \quad 1 \quad -\frac{1}{2}\, e^{i \phi} \sqrt{\frac{15}{2\pi}}\ \mathrm{Cos}[\theta]\ \mathrm{Sin}[\theta]$

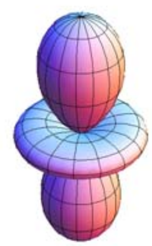
$2 \quad 2 \quad \frac{1}{4}\, e^{2 i \phi} \sqrt{\frac{15}{2\pi}}\ \mathrm{Sin}[\theta]^2$



$l = 2,\ m = \pm 2$



$l = 2,\ m = \pm 1$

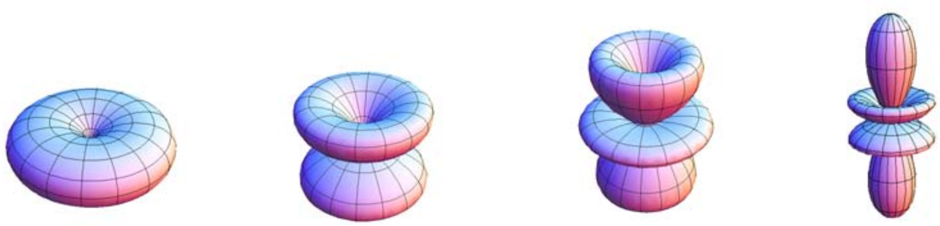


$l = 2,\ m = 0$

(iii) $\langle n | l = 3, m >$ $(m = -3, -2, -1, 0, 1, 2, 3)$

$l$=3 $m$ $Y_{l=3}^{m}(\theta,\phi)$

| | | |
|---|---|---|
| 3 | −3 | $\frac{1}{8} e^{-3 i \phi} \sqrt{\frac{35}{\pi}} \, \mathrm{Sin}[\theta]^3$ |
| 3 | −2 | $\frac{1}{4} e^{-2 i \phi} \sqrt{\frac{105}{2\pi}} \, \mathrm{Cos}[\theta] \, \mathrm{Sin}[\theta]^2$ |
| 3 | −1 | $\frac{1}{16} e^{-i \phi} \sqrt{\frac{21}{\pi}} \, (3 + 5 \, \mathrm{Cos}[2\theta]) \, \mathrm{Sin}[\theta]$ |
| 3 | 0 | $\frac{1}{16} \sqrt{\frac{7}{\pi}} \, (3 \, \mathrm{Cos}[\theta] + 5 \, \mathrm{Cos}[3\theta])$ |
| 3 | 1 | $-\frac{1}{16} e^{i \phi} \sqrt{\frac{21}{\pi}} \, (3 + 5 \, \mathrm{Cos}[2\theta]) \, \mathrm{Sin}[\theta]$ |
| 3 | 2 | $\frac{1}{4} e^{2 i \phi} \sqrt{\frac{105}{2\pi}} \, \mathrm{Cos}[\theta] \, \mathrm{Sin}[\theta]^2$ |
| 3 | 3 | $-\frac{1}{8} e^{3 i \phi} \sqrt{\frac{35}{\pi}} \, \mathrm{Sin}[\theta]^3$ |



$l = 3, m = \pm 3$ $\quad$ $l = 3, m = \pm 2$ $\quad$ $l = 3, m = \pm 1$ $\quad$ $l = 3, m = 0$

## 23.8 Spherical harmonics in the Cartesian coordinate

Using the relation given by

$$x = r \sin\theta \cos\phi, \qquad y = r \sin\theta \sin\phi, \qquad z = r \cos\theta,$$

the spherical harmonics can be expressed as follows,

$$\frac{x}{r} = \sqrt{\frac{2\pi}{3}}[Y_1^{-1}(\theta,\phi) - Y_1^1(\theta,\phi)]$$

$$\frac{y}{r} = i\sqrt{\frac{2\pi}{3}}[Y_1^1(\theta,\phi) + Y_1^{-1}(\theta,\phi)]$$

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

$$-\left(\frac{x+iy}{\sqrt{2}r}\right) = \sqrt{\frac{4\pi}{3}}Y_1^1(\theta,\phi)$$

$$\frac{x-iy}{\sqrt{2}r} = \sqrt{\frac{4\pi}{3}}Y_1^{-1}(\theta,\phi)$$

$$\frac{(x+iy)^2}{r^2} = 4\sqrt{\frac{2\pi}{15}}Y_2^2(\theta,\phi)$$

$$\frac{z(x+iy)}{r^2} = -2\sqrt{\frac{2\pi}{15}}Y_2^1(\theta,\phi)$$

$$\frac{2z^2-(x^2+y^2)}{r^2} = 4\sqrt{\frac{\pi}{5}}Y_2^0(\theta,\phi)$$

$$\frac{z(x-iy)}{r^2} = 2\sqrt{\frac{2\pi}{15}}Y_2^{-1}(\theta,\phi)$$

$$\frac{(x-iy)^2}{r^2} = 4\sqrt{\frac{2\pi}{15}}Y_2^2(\theta,\phi)$$

$$\frac{zx}{r^2} = \sqrt{\frac{2\pi}{15}}[-Y_2^1(\theta,\phi) + Y_2^{-1}(\theta,\phi)]$$

$$\frac{yz}{r^2} = i\sqrt{\frac{2\pi}{15}}[Y_2^1(\theta,\phi) + Y_2^{-1}(\theta,\phi)]$$

$$\frac{xy}{r^2} = -i\sqrt{\frac{2\pi}{15}}[Y_2^2(\theta,\phi) - Y_2^{-2}(\theta,\phi)]$$

## 23.9 Example-1

**((Sakurai 3-15))** The wave function of a particle subjected to a spherically symmetrical potential $V(r)$ is given by

$$\psi(\mathbf{r}) = (x + y + z) f(r)$$

(a) Is $\psi(\mathbf{r})$ an eigenfunction of $\boldsymbol{L}^2$? If so, what is the $l$-value? If not, what are the possible values of $l$ we may obtain when $\boldsymbol{L}^2$ is measured?

(b) What are the probabilities for the particle to be found in various $m$ states?

Noting that

$$\frac{x}{r} = \sqrt{\frac{2\pi}{3}}[Y_1^{-1}(\theta,\phi) - Y_1^{1}(\theta,\phi)]$$

$$\frac{y}{r} = i\sqrt{\frac{2\pi}{3}}[Y_1^{1}(\theta,\phi) + Y_1^{-1}(\theta,\phi)]$$

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

we have

$$\frac{x+y+z}{r} = \sqrt{\frac{2\pi}{3}}[(1+i)Y_1^{-1}(\theta,\phi) - (1-i)Y_1^{1}(\theta,\phi) + \sqrt{2}Y_1^{0}(\theta,\phi)]$$

Then $\psi(\mathbf{r})$ can be rewritten as

$$\psi(x,y,z) = \sqrt{\frac{2\pi}{3}}[(1+i)Y_1^{-1}(\theta,\phi) - (1-i)Y_1^{1}(\theta,\phi) + \sqrt{2}Y_1^{0}(\theta,\phi)]rf(r)$$

This implies that

$$\left|\psi\right\rangle = \frac{1}{\sqrt{6}}[-(1-i)\left|1,1\right\rangle + \sqrt{2}\left|1,0\right\rangle + (1+i)\left|1,-1\right\rangle]$$

So we get

$$\mathbf{L}^2\left|\psi\right\rangle = \hbar^2 l(l+1)\left|\psi\right\rangle$$

with $l = 1$.

$$P(l=1,m) = \left|\langle m|\psi\rangle\right|^2 = \frac{1}{3},$$

which is independent of *m*.

## 23.9 Example-2

A particle moving in a potential is described by the wave packet

$$\psi(r) = (xy + yz + zx)\exp[-\alpha^2(x^2 + y^2 + z^2)]$$

What is the probability that a measurement of $\boldsymbol{L}^2$ and $L_z$ yields the results $6\hbar^2$ and $\hbar$, respectively?

((**Solution**))

We note that

$$\frac{zx}{r^2} = \sqrt{\frac{2\pi}{15}}[-Y_2^1(\theta,\phi) + Y_2^{-1}(\theta,\phi)]$$

$$\frac{yz}{r^2} = i\sqrt{\frac{2\pi}{15}}[Y_2^1(\theta,\phi) + Y_2^{-1}(\theta,\phi)]$$

$$\frac{xy}{r^2} = -i\sqrt{\frac{2\pi}{15}}[Y_2^2(\theta,\phi) - Y_2^{-2}(\theta,\phi)]$$

Then we have

$$\frac{xy + yz + zx}{r^2} = \sqrt{\frac{2\pi}{15}}[-Y_2^1(\theta,\phi) + Y_2^{-1}(\theta,\phi)] + i\sqrt{\frac{2\pi}{15}}[Y_2^1(\theta,\phi) + Y_2^{-1}(\theta,\phi)]$$

$$-i\sqrt{\frac{2\pi}{15}}[Y_2^2(\theta,\phi) - Y_2^{-2}(\theta,\phi)]$$

or

$$\frac{xy + yz + zx}{r^2} = \sqrt{\frac{2\pi}{15}}[(-1+i)Y_2^1(\theta,\phi) + (1+i)Y_2^{-1}(\theta,\phi) - iY_2^2(\theta,\phi) + iY_2^{-2}(\theta,\phi)i]$$

Thus the wave function can be rewritten as

$$\psi(x,y,z)=\sqrt{\frac{2\pi}{15}}[(-1+i)Y_2^1(\theta,\phi)+(1+i)Y_2^{-1}(\theta,\phi)-iY_2^2(\theta,\phi)+iY_2^{-2}(\theta,\phi)]r^2e^{-\alpha r^2}$$

or

$$|\psi\rangle=\frac{1}{\sqrt{6}}[-i|2,2\rangle+(-1+i)|2,1\rangle+(1+i)|2,-1\rangle+i|2,-2\rangle]$$

The probability that a measurement of $\boldsymbol{L}^2$ and $L_z$ yields the results $6\hbar^2$ and $\hbar$, respectively ($l = 2$, $m = 1$) is

$$P=|\langle 2,1|\psi\rangle|^2=\left|\frac{-1+i}{\sqrt{6}}\right|^2=\frac{1}{3}$$

---

**APPENDIX**

**A.1 Mathematica**

1. Legendre polynomial: Legendre$P[n,x]$

2. Associated Ledendre polynomial: Legendre$P[n,m,x]$

 Note that the associated Legendre polynomials are defined by

$$P_l^m(x)=(-1)^m(1-x^2)^{m/2}\frac{d^m}{dx^m}P_l(x) \qquad \text{for } m\geq 0.$$

in the Mathematica.

3. Spherical Harmonics: SphericalHarmonicY[l,m,$\theta$,$\phi$]

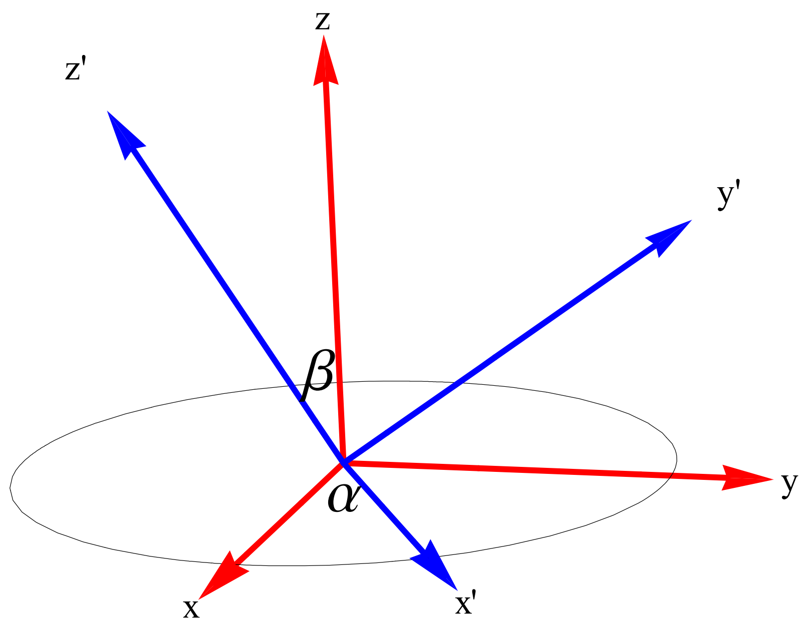
Note that the spherical harmonics is defined by

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

in the Mathematica.

4. SphericalPlot3D[$r$, $\theta$, $\phi$]
 to generates a 3D plot with a spherical radius $r$ as a function of spherical coordinates $\theta$ and $\phi$.

**A.2 Addition theorem for spherical harmonics**




We consider the two coordinate systems, *xyz*, and *x'y'z'*. The position vectors has angular coordinates $\theta$, $\phi$, and $\theta$ and $\phi'$ in the two coordinate systems.

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

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

Under the rotation, an eigenket $|l, m\rangle$ transforms into an eigenket $|l, m\rangle'$, where the *z'* is the axis obtained by the rotation from the *z* axis,

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

and

$$\langle \theta', \phi' | l, m' \rangle' = \sum_{m'} \langle \theta, \phi | l, m' \rangle D_{m',m}^{(l)}(\hat{R})$$

or

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

Using the unitary property of the representation,

$$\begin{aligned}
|l,m\rangle = \hat{R}^{+}|l,m\rangle' &= \sum_{m'}|l,m'\rangle''\langle l,m'|\hat{R}^{+}|l,m\rangle' \\
&= \sum_{m'}|l,m'\rangle'\langle l,m'|\hat{R}\hat{R}^{+}\hat{R}^{+}|l,m\rangle \\
&= \sum_{m'}|l,m'\rangle'\langle l,m'|\hat{R}^{+}|l,m\rangle \\
&= \sum_{m'}|l,m'\rangle'\langle l,m|\hat{R}|l,m'\rangle^{*} \\
&= \sum_{m'}|l,m'\rangle' D_{m,m'}^{(l)\,*}(\hat{R})
\end{aligned}$$

$$\langle\theta,\phi|l,m\rangle = \sum_{m'}\langle\theta',\phi'|l,m'\rangle D_{m,m'}^{(l)\,*}(\hat{R})$$

or

$$Y_l^m(\theta,\phi) = \sum_{m'} Y_l^m(\theta',\phi') D_{m,m'}^{(l)\,*}(\hat{R})$$

We consider in a particular point on the new $z'$ axis,

$$D_{m,0}^{(l)}(\hat{R}) = \sqrt{\frac{4\pi}{2l+1}}\, Y_l^{m^*}(\beta,\alpha).$$

The direction of $z'$ axis in space is specified by its polar angle $\beta$ and its azimuth $\alpha$ with respect to the unprimed system.

$$\begin{aligned}
Y_l^0(\theta',\phi') &= \sum_{m'} Y_l^{m'}(\theta,\phi) D_{m',0}^{(l)}(\hat{R}) \\
&= \sqrt{\frac{4\pi}{2l+1}} \sum_{m'} Y_l^{m'}(\theta,\phi) Y_l^{m^*}(\beta,\alpha)
\end{aligned}$$

or

$$Y_l^0(\theta',\phi') = \sqrt{\frac{2l+1}{4\pi}} P_l(\cos\theta') = \sqrt{\frac{4\pi}{2l+1}} \sum_{m'} Y_l^{m'}(\theta,\phi) Y_l^{m^*}(\beta,\alpha).$$

We finally obtain the additional theorem for spherical harmonics,

$$P_l(\cos\theta') = \frac{4\pi}{2l+1} \sum_{m'} Y_l^{m'}(\theta,\phi) Y_l^{m^*}(\beta,\alpha).$$

## REFERENCE

E. Merzbacher, *Quantum Mechanics*, 3rd edition (John Wiley & Sons, New York, 1998).