# Spherical Harmonics in Quantum mechanics

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Here we discuss the properties of spherical harmonics.

Spherical harmonics
Dirac delta function
Recurrence relation
Associated Legendre functions
Parity
Time reversal operator
SphericalPlot3D
ContourPlot3D
Series expansion

## 1. Formulation

The relation between the spherical coordinates and Cartesian coordinates are schematically shown below.

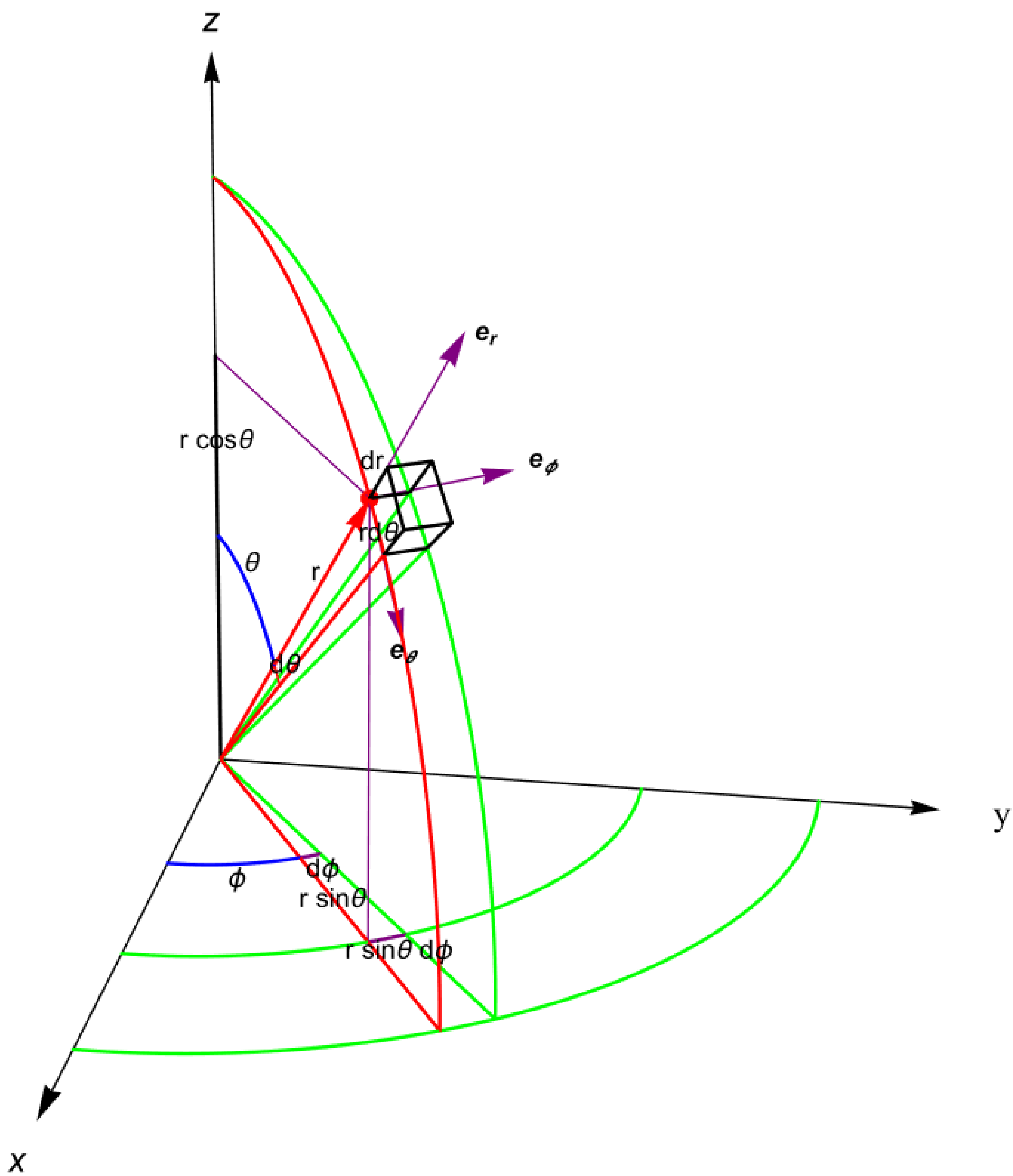



**Fig.1** Spherical coordinates.

$$dV = d^3\mathbf{r} = dr(rd\theta)(r\sin\theta d\phi) = r^2 dr \sin\theta d\theta d\phi = r^2 dr d\Omega \,.$$

The spherical harmonics:

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

where

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

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:

$$\int|\theta,\phi\rangle d\Omega\langle\theta,\phi| = \hat{1} , \qquad \text{or} \qquad \int|\mathbf{n}\rangle d\Omega\langle\mathbf{n}| = \hat{1}$$

where the solid angle,

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

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

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

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

Equation (2) shows that

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

It is required that the eigenfunction must be single valued

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

which means that $m = 0, \pm1, \pm2,$ (integers). Equation (1) can be rewritten as

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

When we change the variable;

$$x = \cos\theta \qquad (|x| \le 1).$$

$$\frac{d}{d\theta} = \frac{dx}{d\theta}\frac{d}{dx} = -\sin\theta \frac{d}{dx}$$

Then we have the differential equation (the Legendre differential equation) as

$$\frac{d}{dx}(1-x^2)\frac{d}{dx}P_l^m(x) + [l(l+1) - \frac{m^2}{1-x^2}]P_l^m(x) = 0 .$$

where $P_l^m(x)$ is the associated Legendre function;

$$\Theta_l^m(\theta) = C_{lm}P_l^m(\cos\theta) .$$

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

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

Note that this differential equation (Sturm-Liouville type) can be solved by using the series expansion method (see later).

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.

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

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 $Y_l^{-m}(\theta,\phi)$ ($m \geq 0$) by

$$Y_l^{-m}(\theta,\phi) = (-1)^m [Y_l^m(\theta,\phi)]^*, \qquad \text{for } m \geq 0,$$

or

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

where somewhat peculiar choice of sign is conventional. The definition of $Y_l^{-m}(\theta,\phi)$ with $m \geq 0$ arises from the property of time-reversal operator;

$$\hat{\Theta}|l,m\rangle = (-1)^m |l,-m\rangle, \qquad \text{or} \qquad |l,-m\rangle = (-1)^m \hat{\Theta}|l,m\rangle$$

where $\hat{\Theta}$ is the time-reversal operator. We note that

$$\begin{aligned}\langle\theta,\phi|l,-m\rangle &= (-1)^m \langle\theta,\phi|\hat{\Theta}|l,m\rangle \\ &= (-1)^m \langle\theta,\phi|l,m\rangle^*\end{aligned}$$

or

$$Y_l^{-m}(\theta,\phi) = (-1)^m [Y_l^m(\theta,\phi)]^*, \qquad \text{for } m \geq 0,$$

since $\langle\theta,\phi|\hat{\Theta}|l,m\rangle = \langle\theta,\phi|l,m\rangle^*$ from the definition (see the Time reversal operator in the lecture note of Quantum Mechanics, Graduate course),

http://bingweb.binghamton.edu/~suzuki/QM_Graduate/Time_reversal_I_operator.pdf

Angular momentum in spherical coordinate is

$$\begin{aligned}\mathbf{L} &= -i\hbar(\mathbf{r}\times\nabla) \\ &= -i\hbar\mathbf{e}_r r\times(\mathbf{e}_r\frac{\partial}{\partial r}+\mathbf{e}_\theta\frac{1}{r}\frac{\partial}{\partial\theta}+\mathbf{e}_\phi\frac{1}{r\sin\theta}\frac{\partial}{\partial\phi}) \\ &= i\hbar(-\mathbf{e}_\phi\frac{\partial}{\partial\theta}+\mathbf{e}_\theta\frac{1}{\sin\theta}\frac{\partial}{\partial\phi})\end{aligned}$$

The angular momentum $L_x$, $L_y$, and $L_z$ (Cartesian components) can be described by

$$\mathbf{L} = i\hbar[-(-\sin\phi\mathbf{e_x}+\cos\phi\mathbf{e}_y)\frac{\partial}{\partial\theta}+(\cos\theta\cos\phi\mathbf{e_x}+\cos\theta\sin\phi\mathbf{e}_y-\sin\theta\mathbf{e}_z)\frac{1}{\sin\theta}\frac{\partial}{\partial\phi}].$$

or

$$L_x = i\hbar(\sin\phi\frac{\partial}{\partial\theta}+\cot\theta\cos\phi\frac{\partial}{\partial\phi}),$$

$$L_y = i\hbar(-\cos\phi\frac{\partial}{\partial\theta}+\cot\theta\sin\phi\frac{\partial}{\partial\phi}),$$

$$L_z = -i\hbar\frac{\partial}{\partial\phi}.$$

We define $L_+$ and $L_-$ as

$$L_+ = L_x + iL_y = -i\hbar e^{i\phi}(i\frac{\partial}{\partial\theta}-\cot\theta\frac{\partial}{\partial\phi}),$$

and

$$L_- = L_x - iL_y = -i\hbar e^{-i\phi}(-i\frac{\partial}{\partial\theta}-\cot\theta\frac{\partial}{\partial\phi}).$$

## 2. Dirac delta function

The Dirac delta function can be described by

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

since

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

Here, we note that

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

where we use the addition theorem

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

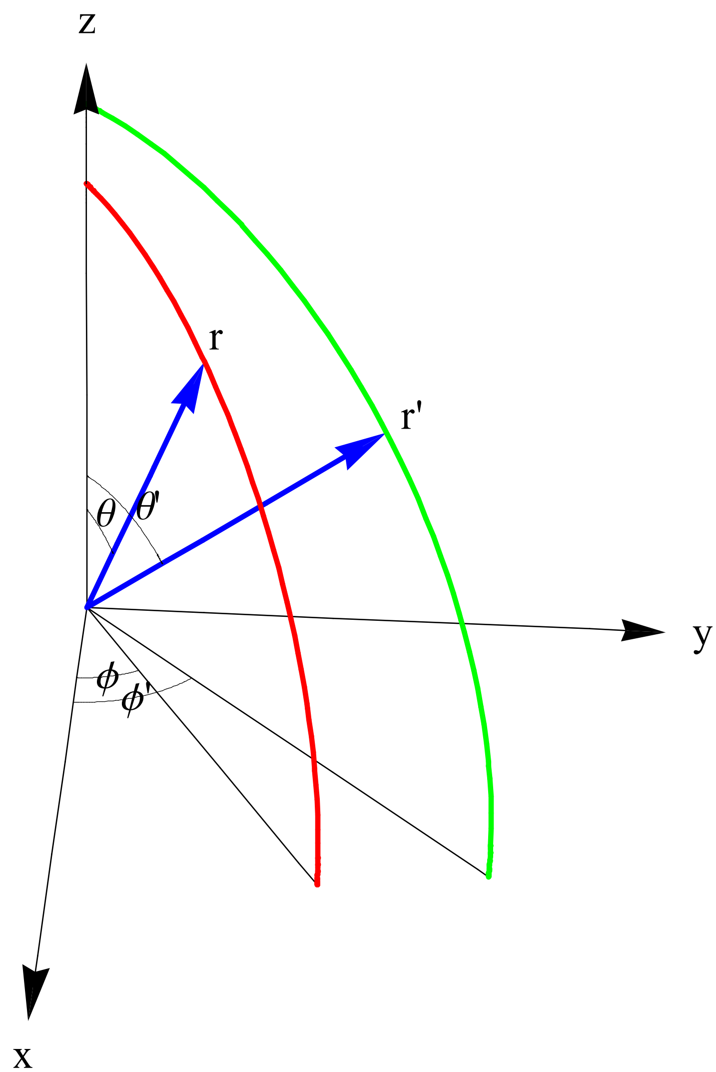



**Fig.2** Angle $\gamma$ such that $\mathbf{n}\cdot\mathbf{n}' = \dfrac{\mathbf{r}\cdot\mathbf{r}'}{rr'} = \cos\gamma$

In summary, the Dirac delta function is expressed by

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

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

((**Note**))

$P_l(x)$ is the $l$-th Legendre polynomial which is defined by the Rodrigues formula

## 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.

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

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

The Rodrigues' formula:

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

$$P_l(1)=1,$$

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

and

$$(l+1)P_{l+1}(x)=(2l+1)xP_l(x)-lP_{l-1}(x)$$

where

$$P_0(x)=1,$$
$$P_1(x)=x,$$
$$P_2(x)=\frac{1}{2}(3x^2-1),$$
$$P_3(x)=\frac{1}{2}(5x^3-3x),$$
$$P_4(x)=\frac{1}{8}(35x^4-30x^2+3),$$

$$P_5(x) = \frac{1}{8}(63x^5 - 70x^3 + 15x)$$

## 4. Parity operator $\hat{\pi}$

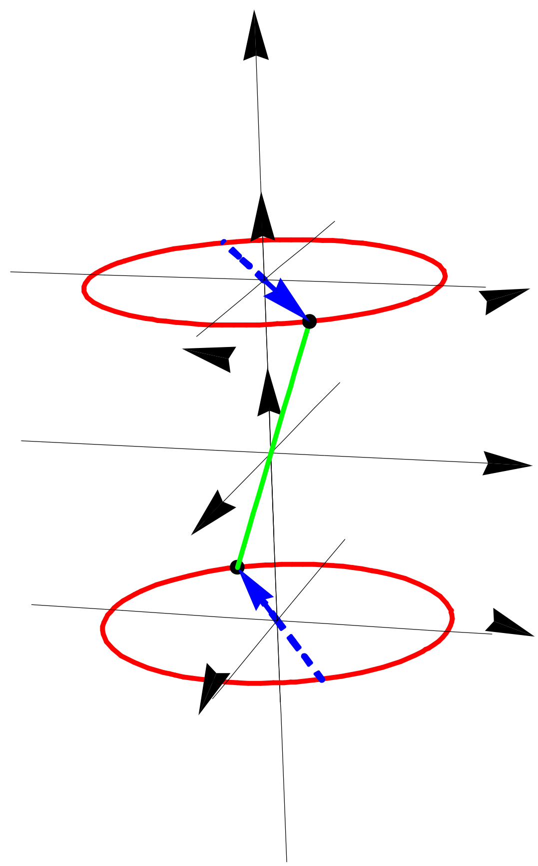


**Fig.3** Space reflection on parity. $\theta \to \pi - \theta$. $\phi \to \pi + \phi$.

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

For $\boldsymbol{n}$ to $-\boldsymbol{n}$, we have

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

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

or

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

((**Note-1**))

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

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

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

when $\theta \to \pi - \theta$. Therefore, we have

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

((**Note-2**)) ((**Binney**))

We start with

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

We note that

$$\begin{aligned}\langle\theta,\phi|\hat{\pi}|l,m=l\rangle &= \langle\pi-\theta,\phi+\pi|l,m=l\rangle \\ &= Y_l^l(\pi-\theta,\phi+\pi) \\ &= C_l e^{il(\phi+\pi)}\sin^l(\pi-\theta) \\ &= e^{\pi il}e^{il\phi}\sin^l(\theta) \\ &= (-1)^l\langle\theta,\phi|l,m=l\rangle\end{aligned}$$

or

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

In other words, $|l,m=l\rangle$ has an even parity if $l$ is an even number and odd parity if $l$ is an odd number.

The ladder operators $\hat{L}_\pm = \hat{L}_x \pm i\hat{L}_y$ are even parity operators;

$$[\hat{\pi},\hat{L}_\pm] = 0 .$$

We use the relation

$$\hat{L}_-|l,m\rangle = \sqrt{(l+m)(l-m+1)}|l,m-1\rangle ,$$

$$\hat{L}_+|l,m\rangle = \sqrt{(l-m)(l+m+1)}|l,m+1\rangle .$$

We apply the parity operator to $|l,m=l-1\rangle$.

$$\hat{\pi}|l,m=l-1\rangle = \hat{\pi}\frac{1}{\sqrt{2l}}\hat{L}_-|l,m=l\rangle = \frac{1}{\sqrt{2l}}\hat{L}_-\hat{\pi}|l,m=l\rangle = \frac{1}{\sqrt{2l}}\hat{L}_-(-1)^l|l,m=l\rangle$$

or

$$\hat{\pi}|l,m=l-1\rangle = (-1)^l\frac{1}{\sqrt{2l}}\hat{L}_-|l,m=l\rangle = (-1)^l|l,m=l-1\rangle$$

So that $|l, m = l-1\rangle$ has the same parity as $|l, m = l-1\rangle$. Since all the $|l, m\rangle$ for a given $l$ can be obtained by repeated application of $\hat{L}_-$ to $|l, m = l\rangle$, it follows that they all have the same parity, $(-1)^l$.

## 5. Determination of the parity with the use of Mathematica

We evaluate the parity

$$\frac{Y_l^m(\pi-\theta, \phi+\pi)}{Y_l^m(\theta, \phi)},$$

as a function of $(l, m)$.

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

((**Mathematica-1**))

Table of $\{l, m, \text{the parity}\}$; the parity is assumed to be $(-1)^l$. We make sure of this prediction using the Mathematica.

```
Clear["Global`*"];
P[L_, m_] := SphericalHarmonicY[L, m, π - θ, ϕ + π] / SphericalHarmonicY[L, m, θ, ϕ] //
  Simplify;

Column[Table[{L, m, P[L, m]}, {L, 0, 5},
  {m, -L, L, 1}], Left]

{{0, 0, 1}}
{{1, -1, -1}, {1, 0, -1}, {1, 1, -1}}
{{2, -2, 1}, {2, -1, 1}, {2, 0, 1}, {2, 1, 1}, {2, 2, 1}}
{{3, -3, -1}, {3, -2, -1}, {3, -1, -1},
 {3, 0, -1}, {3, 1, -1}, {3, 2, -1}, {3, 3, -1}}
{{4, -4, 1}, {4, -3, 1}, {4, -2, 1}, {4, -1, 1},
 {4, 0, 1}, {4, 1, 1}, {4, 2, 1}, {4, 3, 1}, {4, 4, 1}}
{{5, -5, -1}, {5, -4, -1}, {5, -3, -1},
 {5, -2, -1}, {5, -1, -1}, {5, 0, -1}, {5, 1, -1},
 {5, 2, -1}, {5, 3, -1}, {5, 4, -1}, {5, 5, -1}}
```

## 6. Recurrence relation

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

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

where $P_l(\cos\theta)$ is the Legendre polynomial.

We can find the exact expressions for the spherical harmonics using the above recurrence relation, using the Mathematica. We can make sure that

$$Y_l^{-m}(\theta,\phi) = (-1)^m[Y_l^m(\theta,\phi)]^* \qquad \text{for } m \geq 0.$$

((**Mathematica-2**))

l = 0, m = 0

```
Table[{0, m, SphericalHarmonicY[0, m,
     θ, ϕ] },
   {m, 0, 0, 0}] // Simplify // TableForm
```

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

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

```
Table[{1, m, 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[$\theta$] |
| 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 = 2, m = 2, 1, 0, -1, -2

```
Table[{2, n, SphericalHarmonicY[2, n,
     θ, ϕ]}, {n, 2, -2, -1}] // Simplify //
 TableForm
```

| | | |
|---|---|---|
| 2 | 2 | $\frac{1}{4} e^{2 i \phi} \sqrt{\frac{15}{2\pi}} \mathrm{Sin}[\theta]^2$ |
| 2 | 1 | $-\frac{1}{2} e^{i \phi} \sqrt{\frac{15}{2\pi}} \mathrm{Cos}[\theta]\, \mathrm{Sin}[\theta]$ |
| 2 | 0 | $\frac{1}{8} \sqrt{\frac{5}{\pi}} (1 + 3\, \mathrm{Cos}[2\theta])$ |
| 2 | -1 | $\frac{1}{2} e^{-i \phi} \sqrt{\frac{15}{2\pi}} \mathrm{Cos}[\theta]\, \mathrm{Sin}[\theta]$ |
| 2 | -2 | $\frac{1}{4} e^{-2 i \phi} \sqrt{\frac{15}{2\pi}} \mathrm{Sin}[\theta]^2$ |

l = 3, m = 3, 2, 1, 0, -1, -2, -3

```
Table[{3, m, SphericalHarmonicY[3, m,
    θ, ϕ]}, {m, 3, -3, -1}] // Simplify //
 TableForm
```

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

l = 4, m = 4, 3, 2, 1, 0, -1, -2, -3, -4

```
Table[{4, m, SphericalHarmonicY[4, m, θ, ϕ]},
  {m, 4, -4, -1}] // Simplify // TableForm
```

| | | |
|---|---|---|
| 4 | 4 | $\frac{3}{16} e^{4 i \phi} \sqrt{\frac{35}{2\pi}} \operatorname{Sin}[\theta]^4$ |
| 4 | 3 | $-\frac{3}{8} e^{3 i \phi} \sqrt{\frac{35}{\pi}} \operatorname{Cos}[\theta] \operatorname{Sin}[\theta]^3$ |
| 4 | 2 | $\frac{3}{16} e^{2 i \phi} \sqrt{\frac{5}{2\pi}} (5 + 7 \operatorname{Cos}[2\theta]) \operatorname{Sin}[\theta]^2$ |
| 4 | 1 | $-\frac{3}{32} e^{i \phi} \sqrt{\frac{5}{\pi}} (1 + 7 \operatorname{Cos}[2\theta]) \operatorname{Sin}[2\theta]$ |
| 4 | 0 | $\frac{3 (9 + 20 \operatorname{Cos}[2\theta] + 35 \operatorname{Cos}[4\theta])}{128 \sqrt{\pi}}$ |
| 4 | -1 | $\frac{3}{32} e^{-i \phi} \sqrt{\frac{5}{\pi}} (1 + 7 \operatorname{Cos}[2\theta]) \operatorname{Sin}[2\theta]$ |
| 4 | -2 | $\frac{3}{16} e^{-2 i \phi} \sqrt{\frac{5}{2\pi}} (5 + 7 \operatorname{Cos}[2\theta]) \operatorname{Sin}[\theta]^2$ |
| 4 | -3 | $\frac{3}{8} e^{-3 i \phi} \sqrt{\frac{35}{\pi}} \operatorname{Cos}[\theta] \operatorname{Sin}[\theta]^3$ |
| 4 | -4 | $\frac{3}{16} e^{-4 i \phi} \sqrt{\frac{35}{2\pi}} \operatorname{Sin}[\theta]^4$ |

## 7. Useful formula (summary)

**(i)**

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

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

**(ii)** 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

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

**(iii)**

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

**(iv)**

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

**(v)**

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

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

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

or

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

**(vi)**

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

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

or

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

We also have

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

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

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

or

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

**(vii)**

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

where we use the addition theorem

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

## 8. Calculation of $D_{m,0}^{(l)}(\hat{R}) = \langle l,m|\hat{R}|l,0\rangle^*$

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

where

$$\hat{R} = \hat{R}_z(\phi)\hat{R}_y(\theta).$$

(a) $l = 1$

$$\langle l=1,m=1|\hat{R}|l=1,m=0\rangle = -\frac{1}{\sqrt{2}}e^{-i\phi}\sin\theta$$

$$\langle l=1,m=0|\hat{R}|l=1,m=0\rangle = \cos\theta$$

$$\langle l=1,m=-1|\hat{R}|l=1,m=0\rangle = \frac{1}{\sqrt{2}}e^{i\phi}\sin\theta$$

where

$$Y_1^1(\theta,\phi) = -\frac{1}{2}\sqrt{\frac{3}{2\pi}}e^{i\phi}\sin\theta$$

$$Y_1^0(\theta,\phi) = \frac{1}{2}\sqrt{\frac{3}{\pi}}\cos\theta$$

$$Y_1^{-1}(\theta,\phi) = \frac{1}{2}\sqrt{\frac{3}{2\pi}}e^{-i\phi}\sin\theta$$

(b) $l = 2$

$$\langle l = 2, m = 2|\hat{R}|l = 2, m = 0\rangle = \frac{1}{2}\sqrt{\frac{3}{2}}e^{-2i\phi}\sin^2\theta$$

$$\langle l = 2, m = 1|\hat{R}|l = 2, m = 0\rangle = -\sqrt{\frac{3}{2}}e^{-i\phi}\sin\theta\cos\theta$$

$$\langle l = 2, m = 0|\hat{R}|l = 2, m = 0\rangle = \frac{1}{4}(1 + 3\cos 2\theta)$$

$$\langle l = 2, m = -1|\hat{R}|l = 2, m = 0\rangle = \sqrt{\frac{3}{2}}e^{i\phi}\sin\theta\cos\theta$$

$$\langle l = 2, m = -2|\hat{R}|l = 2, m = 0\rangle = \frac{1}{2}\sqrt{\frac{3}{2}}e^{2i\phi}\sin^2\theta$$

where

$$Y_2^2(\theta,\phi) = \frac{1}{4}\sqrt{\frac{15}{2\pi}}e^{i2\phi}\sin^2\theta$$

$$Y_2^1(\theta,\phi) = -\frac{1}{2}\sqrt{\frac{15}{2\pi}}e^{i\phi}\sin\theta\cos\theta$$

$$Y_2^0(\theta,\phi) = \frac{1}{4}\sqrt{\frac{5}{\pi}}(3\cos^2\theta - 1)$$

$$Y_2^{-1}(\theta,\phi) = \frac{1}{2}\sqrt{\frac{15}{2\pi}}e^{-i\phi}\sin\theta\cos\theta$$

$$Y_2^{-2}(\theta,\phi) = \frac{1}{4}\sqrt{\frac{15}{2\pi}}e^{-i2\phi}\sin^2\theta$$

(c) $l = 3$

$$\langle l=3, m=3|\hat{R}|l=3, m=0\rangle = -\frac{1}{4}\sqrt{5}e^{-3i\phi}\sin^3\theta .$$

$$\langle l=3, m=2|\hat{R}|l=3, m=0\rangle = \frac{1}{2}\sqrt{\frac{15}{2}}e^{-2i\phi}\sin^2\theta\cos\theta .$$

$$\langle l=3, m=1|\hat{R}|l=3, m=0\rangle = -\frac{1}{16}\sqrt{3}e^{-i\phi}(\sin\theta + 5\sin 3\theta) .$$

$$\langle l=3, m=0|\hat{R}|l=3, m=0\rangle = \frac{1}{8}(3\cos\theta + 5\cos 3\theta) .$$

$$\langle l=3, m=-1|\hat{R}|l=3, m=0\rangle = \frac{1}{16}\sqrt{3}e^{i\phi}(\sin\theta + 5\sin 3\theta) .$$

$$\langle l=3, m=-2|\hat{R}|l=3, m=0\rangle = \frac{1}{2}\sqrt{\frac{15}{2}}e^{2i\phi}\sin^2\theta\cos\theta .$$

$$\langle l=3, m=-3|\hat{R}|l=3, m=0\rangle = \frac{1}{4}\sqrt{5}e^{3i\phi}\sin^3\theta .$$

where

$$Y_3^3(\theta,\phi) = -\frac{1}{8}\sqrt{\frac{35}{\pi}}e^{i3\phi}\sin^3\theta .$$

$$Y_3^2(\theta,\phi) = \frac{1}{4}\sqrt{\frac{105}{2\pi}}e^{i2\phi}\sin^2\theta\cos\theta .$$

$$Y_3^1(\theta,\phi) = -\frac{1}{8}\sqrt{\frac{21}{\pi}}e^{i\phi}\sin\theta(5\cos^2\theta - 1) .$$

$$Y_3^0(\theta,\phi) = \frac{1}{4}\sqrt{\frac{7}{\pi}}(5\cos^3\theta - 3\cos\theta) .$$

$$Y_3^{-1}(\theta,\phi) = \frac{1}{8}\sqrt{\frac{21}{\pi}}e^{-i\phi}\sin\theta(5\cos^2\theta - 1) .$$

$$Y_3^{-2}(\theta,\phi) = \frac{1}{4}\sqrt{\frac{105}{2\pi}} e^{-i2\phi} \sin^2\theta \cos\theta .$$

$$Y_3^{-3}(\theta,\phi) = \frac{1}{8}\sqrt{\frac{35}{\pi}} e^{-i3\phi} \sin^3\theta .$$

(d) $l = 4$

$$\langle l=4, m=4 | \hat{R} | l=4, m=0 \rangle = \frac{1}{8}\sqrt{\frac{35}{2}} e^{-i4\phi} \sin^4\theta .$$

$$\langle l=4, m=3 | \hat{R} | l=4, m=0 \rangle = -\frac{1}{4}\sqrt{35} e^{-i3\phi} \sin^3\theta \cos\theta .$$

$$\langle l=4, m=2 | \hat{R} | l=4, m=0 \rangle = \frac{1}{8}\sqrt{\frac{5}{2}} e^{-i2\phi} [5 + 7\cos(2\theta)] \sin^2\theta .$$

$$\langle l=4, m=1 | \hat{R} | l=4, m=0 \rangle = -\frac{1}{32}\sqrt{5} e^{-i\phi} [2\sin(2\theta) + 7\sin(4\theta)] .$$

$$\langle l=4, m=0 | \hat{R} | l=4, m=0 \rangle = \frac{1}{64} [9 + 20\cos(2\theta) + 35\cos(4\theta)] .$$

$$\langle l=4, m=-1 | \hat{R} | l=4, m=0 \rangle = \frac{1}{32}\sqrt{5} e^{i\phi} [2\sin(2\theta) + 7\sin(4\theta)] .$$

$$\langle l=4, m=-2 | \hat{R} | l=4, m=0 \rangle = \frac{1}{8}\sqrt{\frac{5}{2}} e^{i2\phi} [5 + 7\cos(2\theta)] \sin^2\theta$$

$$\langle l=4, m=-3 | \hat{R} | l=4, m=0 \rangle = \frac{1}{4}\sqrt{35} e^{i3\phi} \sin^3\theta \cos\theta$$

$$\langle l=4, m=-4 | \hat{R} | l=4, m=0 \rangle = \frac{1}{8}\sqrt{\frac{35}{2}} e^{i4\phi} \sin^4\theta$$

where

$$Y_4^{4}(\theta,\phi) = \frac{3}{16}\sqrt{\frac{35}{2\pi}} e^{i4\phi} \sin^4\theta$$

$$Y_4^3(\theta,\phi) = -\frac{3}{8}\sqrt{\frac{35}{\pi}}e^{i3\phi}\sin^3\theta\cos\theta$$

$$Y_4^2(\theta,\phi) = \frac{3}{8}\sqrt{\frac{5}{2\pi}}e^{i2\phi}\sin^2\theta(7\cos^2\theta - 1)$$

$$Y_4^1(\theta,\phi) = -\frac{3}{8}\sqrt{\frac{5}{\pi}}e^{i\phi}\sin\theta(7\cos^3\theta - 3\cos\theta)$$

$$Y_4^0(\theta,\phi) = \frac{3}{16}\sqrt{\frac{1}{\pi}}(35\cos^4\theta - 30\cos^2\theta + 3)$$

$$Y_4^{-1}(\theta,\phi) = \frac{3}{8}\sqrt{\frac{5}{\pi}}e^{-i\phi}\sin\theta(7\cos^3\theta - 3\cos\theta)$$

$$Y_4^{-2}(\theta,\phi) = \frac{3}{8}\sqrt{\frac{5}{2\pi}}e^{-i2\phi}\sin^2\theta(7\cos^2\theta - 1)$$

$$Y_4^{-3}(\theta,\phi) = \frac{3}{8}\sqrt{\frac{35}{\pi}}e^{-i3\phi}\sin^3\theta\cos\theta$$

$$Y_4^{-4}(\theta,\phi) = \frac{3}{16}\sqrt{\frac{35}{2\pi}}e^{-i4\phi}\sin^4\theta$$

See the Table of spherical harmonics (in detail)
http://en.wikipedia.org/wiki/Table_of_spherical_harmonics

## 9. Addition theorem

Let

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

with the geometrical rotation defined by

$$\Re(\theta_1,\phi_1) = \Re_z(\phi_1)\Re_y(\theta_1) = \begin{pmatrix} \cos\theta_1\cos\phi_1 & -\sin\phi_1 & \sin\theta_1\cos\phi_1 \\ \cos\theta_1\sin\phi_1 & \cos\phi_1 & \sin\theta_1\sin\phi_1 \\ -\sin\theta_1 & 0 & \cos\theta_1 \end{pmatrix}$$

$$\Re_z(\phi_1) = \begin{pmatrix} \cos\phi_1 & -\sin\phi_1 & 0 \\ \sin\phi_1 & \cos\phi_1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \qquad \Re_y(\theta_1) = \begin{pmatrix} \cos\theta & 0 & \sin\theta \\ 0 & 1 & 0 \\ -\sin\theta & 0 & \cos\theta \end{pmatrix}$$

The unit vector $\boldsymbol{n}_1$ is defined by

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

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

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

where the geometrical rotation matrix is given by

$$\Re(\theta_2, \phi_2) = \Re_z(\phi_2)\Re_y(\theta_2) = \begin{pmatrix} \cos\theta_2\cos\phi_2 & -\sin\phi_2 & \sin\theta_2\cos\phi_2 \\ \cos\theta_2\sin\phi_2 & \cos\phi_2 & \sin\theta_2\sin\phi_2 \\ -\sin\theta_2 & 0 & \cos\theta_2 \end{pmatrix}$$

Note that

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

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

$$\left|\boldsymbol{n}'\right\rangle = \hat{R}^{-1}(\theta_1,\phi_1)\left|\boldsymbol{n}_2\right\rangle = \left|\Re^{-1}(\theta_1,\phi_1)\boldsymbol{n}_2\right\rangle,$$

and

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

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

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

and

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

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, $\Theta$ is the angle between $\boldsymbol{n}'$ and $\boldsymbol{e}_z$ and it is also the angle between $\mathbf{n}_1$ and $\mathbf{n}_2$.

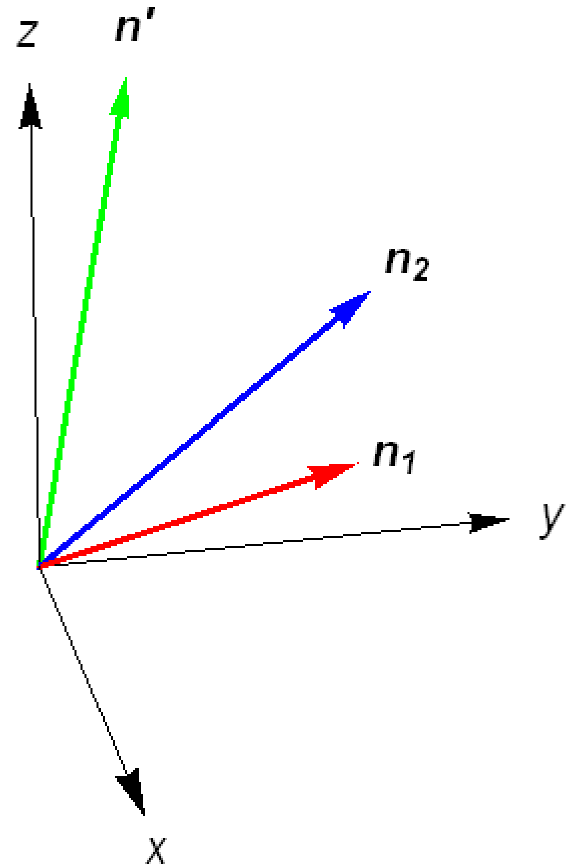



**Fig.4** Three vectors $\mathbf{n}_1 = \Re(\theta_1, \phi_1)\mathbf{e}_z$. $\mathbf{n}_2 = \Re(\theta_2, \phi_2)\mathbf{e}_z$. $\mathbf{n}' = \Re^{-1}(\theta_1, \phi_1)\mathbf{n}_2 = \Re(\Theta, \Phi)\mathbf{e}_z$. The Mathematica is used for this figure. $\theta_1 = 60°$. $\theta_2 = 45°$. $\phi_1 = 30°$. $\phi_2 = 50°$. Without Mathematica, it is hard for me to get the line for the unit vector ***n***'.

Using the closure relation, we get

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

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 $m = 0$;

$$D^{(l)}_{m'm=0}(\theta_1,\phi_1) = e^{-im'\phi_1} d^{(l)}_{m'm=0}(\theta_1)$$

where

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

and

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

Then we have

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

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)**

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

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

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

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

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

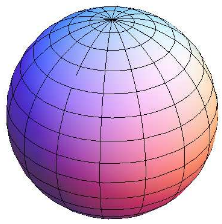
or

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

## 10. SphericalPlot3D of $|Y_l^m(\theta,\phi)|^2$

(i) $\langle \boldsymbol{n}|l=0, m=0\rangle$

$$Y_0^0(\theta,\phi) = \frac{1}{2\sqrt{\pi}}$$



$l = 0$, $m = 0$

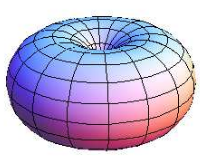
**Fig.5** SphericalPlot3D of $\left|Y_0^0(\theta,\phi)\right|^2$

(ii) $\langle \boldsymbol{n} | l = 1, m \rangle$ ($m$ = 1, 0, -1)

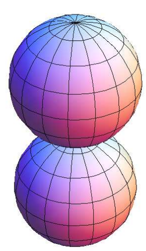
$$Y_1^1(\theta,\phi) = -\frac{1}{2}\sqrt{\frac{3}{2\pi}}e^{i\phi}\sin\theta = -\frac{1}{2}\sqrt{\frac{3}{2\pi}}\frac{(x+iy)}{r},$$

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

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



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



$l = 1$, $m = 0$

**Fig.6** SphericalPlot3D of $\left|Y_1^m(\theta,\phi)\right|^2$ with $m$ = 1, 0, -1.

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

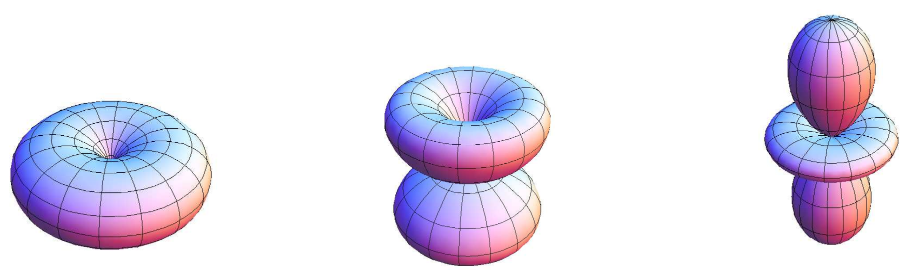
$$Y_2^2(\theta,\phi) = \frac{1}{4}\sqrt{\frac{15}{2\pi}} e^{2i\phi} \sin^2\theta = \frac{1}{4}\sqrt{\frac{15}{2\pi}} \frac{(x+iy)^2}{r^2},$$

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

$$Y_2^0(\theta,\phi) = \frac{1}{8}\sqrt{\frac{5}{\pi}}[1+3\cos(2\theta)] = \frac{1}{4}\sqrt{\frac{5}{\pi}}(3\cos^2\theta - 1) = \frac{1}{4}\sqrt{\frac{5}{\pi}}(\frac{3z^2-r^2}{r^2}),$$

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

$$Y_2^{-2}(\theta,\phi) = \frac{1}{4}\sqrt{\frac{15}{2\pi}} e^{-2i\phi} \sin^2\theta = \frac{1}{4}\sqrt{\frac{15}{2\pi}} \frac{(x-iy)^2}{r^2}.$$



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

**Fig.7** SphericalPlot3D of $\left|Y_2^m(\theta,\phi)\right|^2$ with $m$ = 2, 1, 0, -1, -2.

(iii) $\langle \boldsymbol{n} | l = 3, m \rangle$ ($m$ = 3, 2, 1, 0, -1, -2, -3)

$$Y_3^3(\theta,\phi) = -\frac{1}{8}\sqrt{\frac{35}{\pi}} e^{3i\phi} \sin^3\theta = -\frac{1}{8}\sqrt{\frac{35}{\pi}} \frac{(x+iy)^3}{r^3},$$

$$Y_3^2(\theta,\phi) = \frac{1}{4}\sqrt{\frac{105}{2\pi}} e^{2i\phi} \sin^2\theta\cos\theta = \frac{1}{4}\sqrt{\frac{105}{2\pi}} \frac{z(x+iy)^2}{r^3},$$

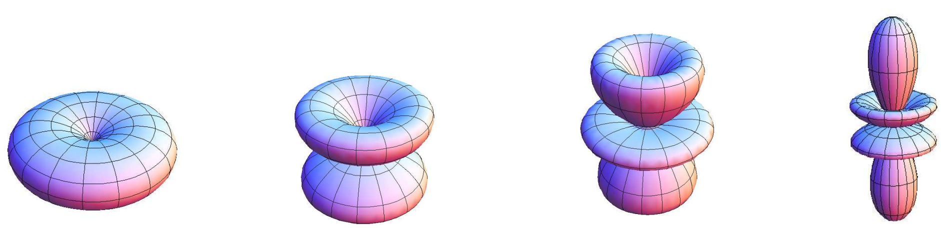
$$Y_3^1(\theta,\phi) = -\frac{1}{16}\sqrt{\frac{21}{\pi}}e^{i\phi}[3+5\cos(2\theta)]\sin\theta$$
$$= -\frac{1}{8}\sqrt{\frac{21}{\pi}}e^{i\phi}(5\cos^2\theta - 1)\sin\theta \quad ,$$
$$= -\frac{1}{8}\sqrt{\frac{21}{\pi}}(\frac{5z^2 - r^2}{r^2})(x+iy)$$

$$Y_3^0(\theta,\phi) = \frac{1}{16}\sqrt{\frac{7}{\pi}}[3\cos\theta + 5\cos(3\theta)$$
$$= \frac{4}{16}\sqrt{\frac{7}{\pi}}\cos\theta(5\cos^2\theta - 3) \ ,$$
$$= \frac{4}{16}\sqrt{\frac{7}{\pi}}\frac{z(5z^2 - 3r^2)}{r^3}$$

$$Y_3^{-1}(\theta,\phi) = \frac{1}{16}\sqrt{\frac{21}{\pi}}e^{-i\phi}[3+5\cos(2\theta)]\sin\theta$$
$$= \frac{1}{8}\sqrt{\frac{21}{\pi}}e^{-i\phi}(5\cos^2\theta - 1)\sin\theta \quad ,$$
$$= \frac{1}{8}\sqrt{\frac{21}{\pi}}(\frac{5z^2 - r^2}{r^2})(x-iy)$$

$$Y_3^{-2}(\theta,\phi) = \frac{1}{4}\sqrt{\frac{105}{2\pi}}e^{-2i\phi}\sin^2\theta\cos\theta = \frac{1}{4}\sqrt{\frac{105}{2\pi}}\frac{z(x-iy)^2}{r^3} \ ,$$

$$Y_3^{-3}(\theta,\phi) = \frac{1}{8}\sqrt{\frac{35}{\pi}}e^{-3i\phi}\sin^3\theta = \frac{1}{8}\sqrt{\frac{35}{\pi}}\frac{(x-iy)^3}{r^3} \ .$$



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

**Fig.8** SphericalPlot3D of $\left|Y_3^m(\theta,\phi)\right|^2$ with $m$ = 3, 2, 1, 0, -1, -2, -3

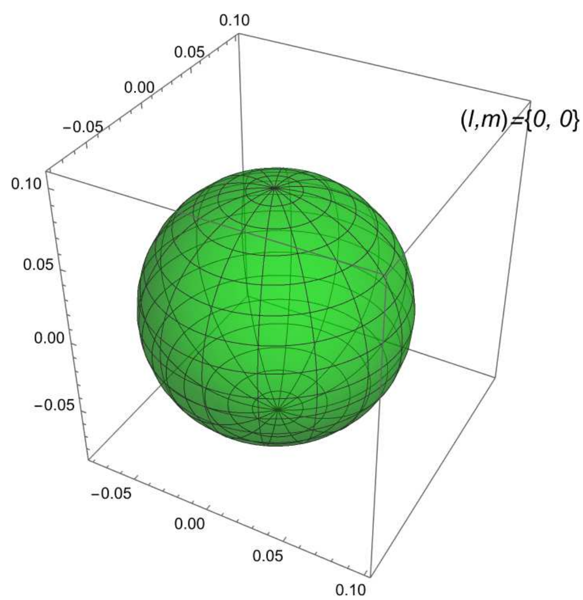
**((Mathematica-3**, **SphericalPlot3D**))

```
Clear["Global`"];
f1[L1_, M1_] :=
 Module[{g1, g2},
  g1 = SphericalPlot3D[Abs[SphericalHarmonicY[L1, M1, θ, ϕ]]^2,
     {θ, 0, π}, {ϕ, 0, 2 π}, PlotRange → All, PlotPoints → 50,
     PlotStyle → {Green, Opacity[0.5]}] // FullSimplify;
  g2 =
   Graphics3D[
    {Text[Style["(l,m)=" <> ToString[{L1, M1}], Black, Italic, 15],
      {0.1, 0.1, 0.10}]}];
  Show[g1, g2]];
```

---

**$l$ = 0 ($m$ =0): SphericalPlot3D**

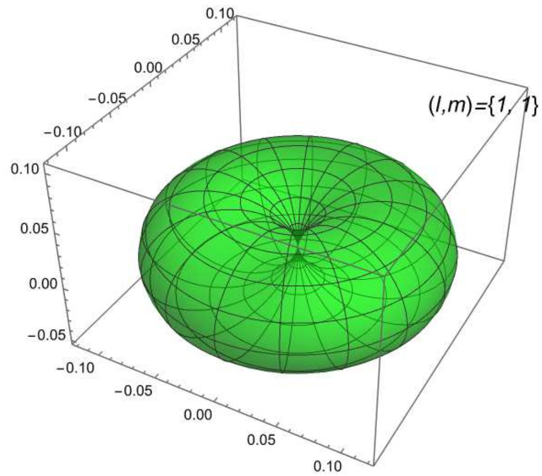
**Fig.9**

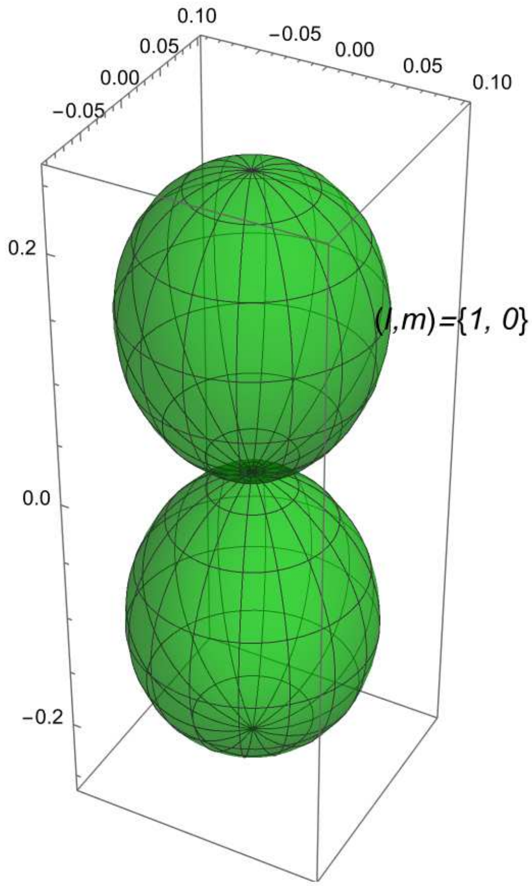



---

**$l$ = 1 ($m$ =1, 0): SphericalPlot3D**

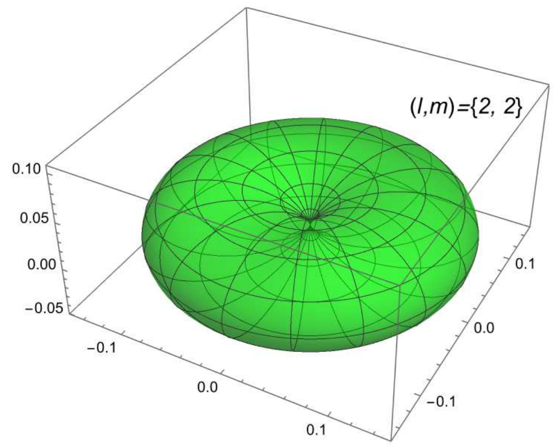
**Fig.10**

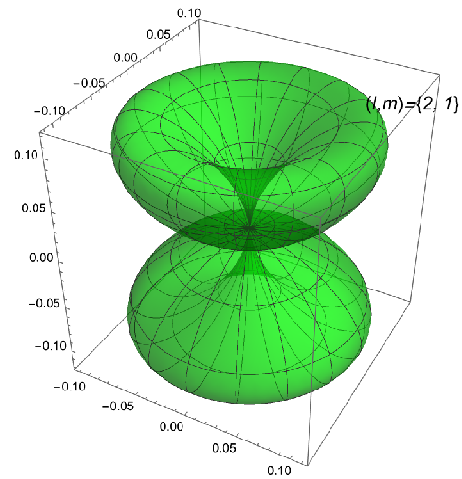


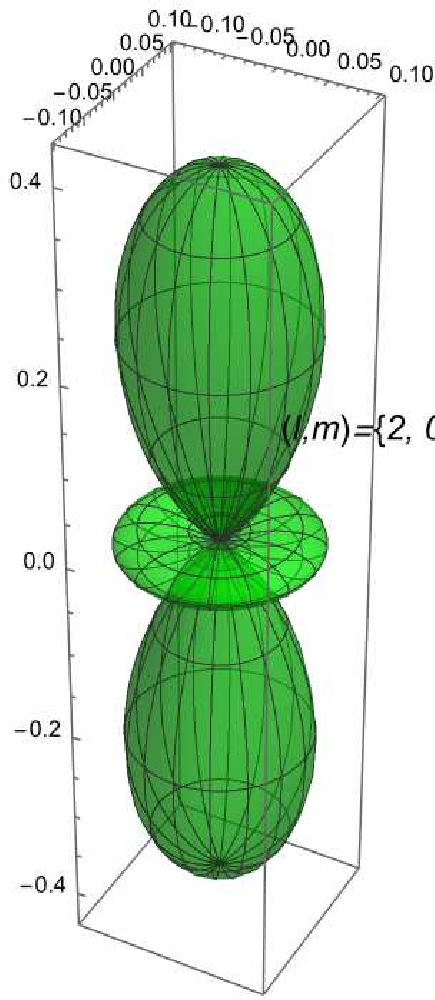




**_l_ = 2 (_m_ =2, 1, 0): SphericalPlot3D**

**Fig.11**

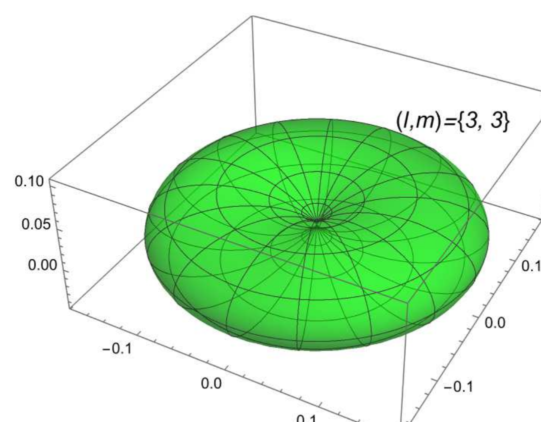

(l,m)={2, 2}
0.10
0.05
0.00
−0.05
−0.1
0.0
0.1
0.1
0.0
−0.1

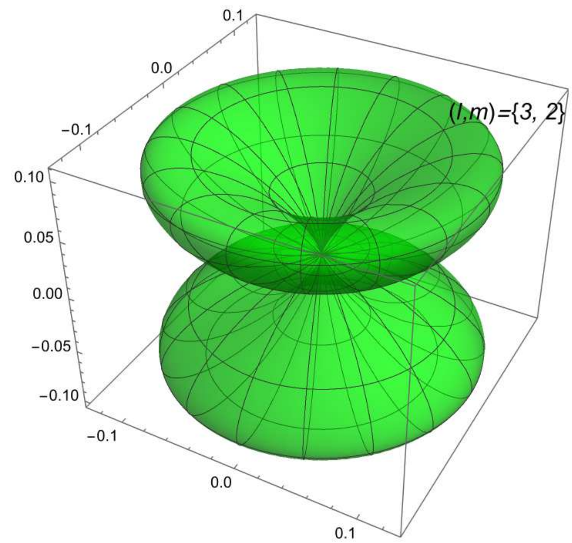

(l,m)={2, 1}
0.10
0.05
0.00
−0.05
−0.10
0.10
0.05
0.00
−0.05
−0.10
−0.10
−0.05
0.00
0.05
0.10

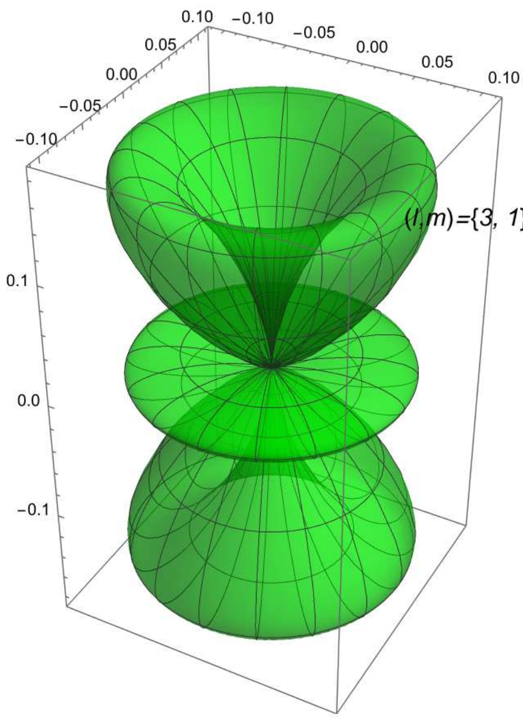


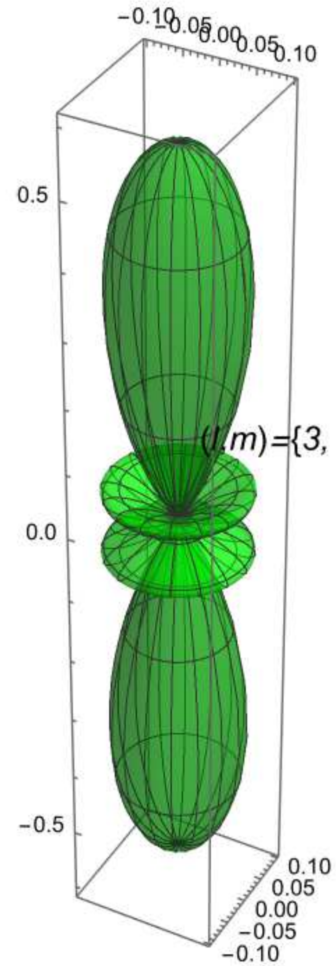

**$l$ = 3 ($m$ = 3, 2, 1, 0): SphericalPlot3D**

**Fig.12**



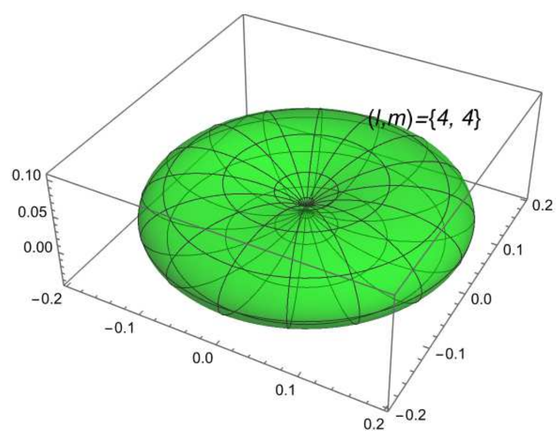

0.1
0.0
−0.1
0.10
0.05
0.00
−0.05
−0.10
−0.1
0.0
0.1
(l,m)={3, 2}

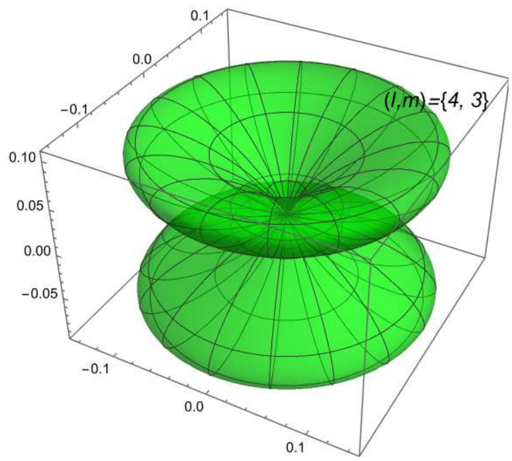

0.10
0.05
0.00
−0.05
−0.10
−0.10
−0.05
0.00
0.05
0.10
0.1
0.0
−0.1
(l,m)={3, 1}

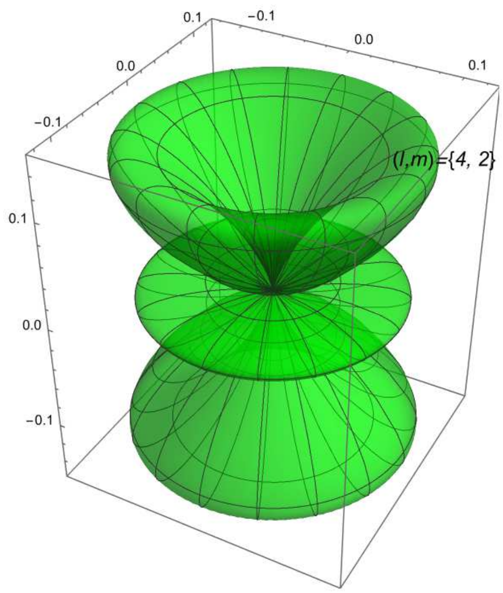


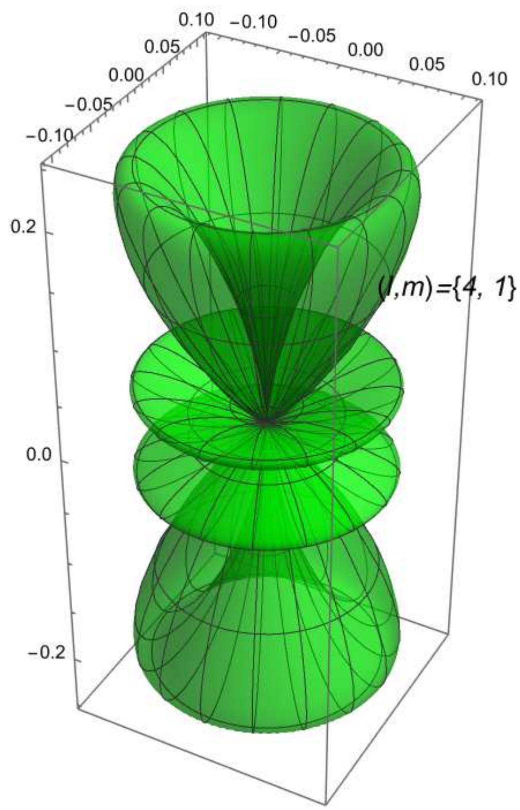

**$l$ = 4 ($m$ =4, 3, 2, 1, 0): SphericalPlot3D**

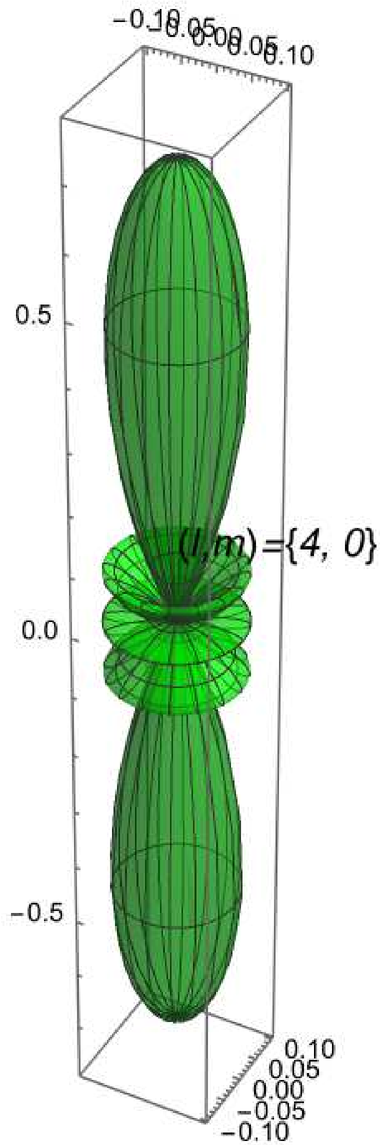
**Fig.13**




(l,m)={4, 3}
0.1
0.0
−0.1
0.10
0.05
0.00
−0.05
−0.1
0.0
0.1

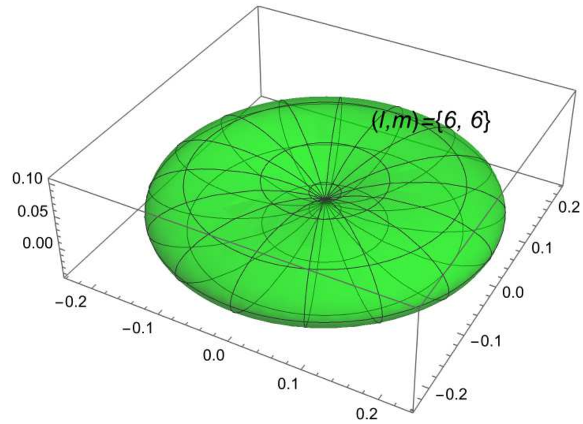

(l,m)={4, 2}
0.1
−0.1
0.0
0.1
0.0
−0.1
0.1
0.0
−0.1

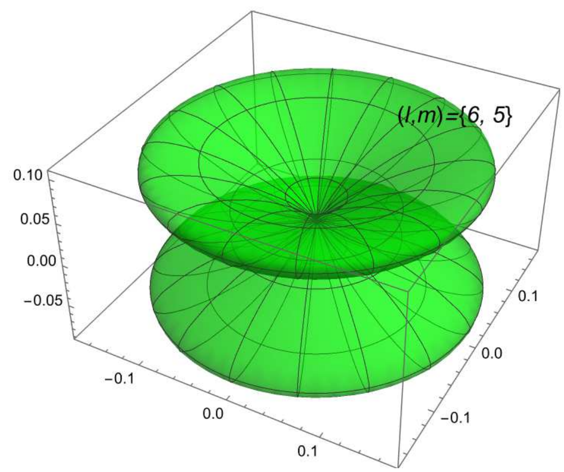

0.10
0.05
0.00
−0.05
−0.10
−0.10
−0.05
0.00
0.05
0.10
0.2
0.0
−0.2
$(l,m)=\{4, 1\}$

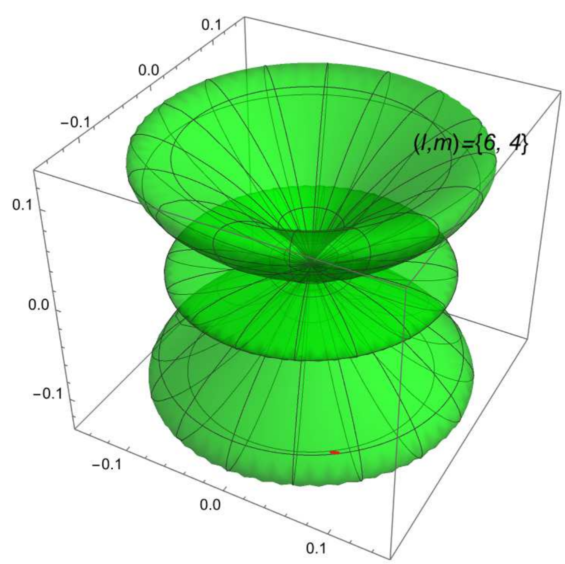


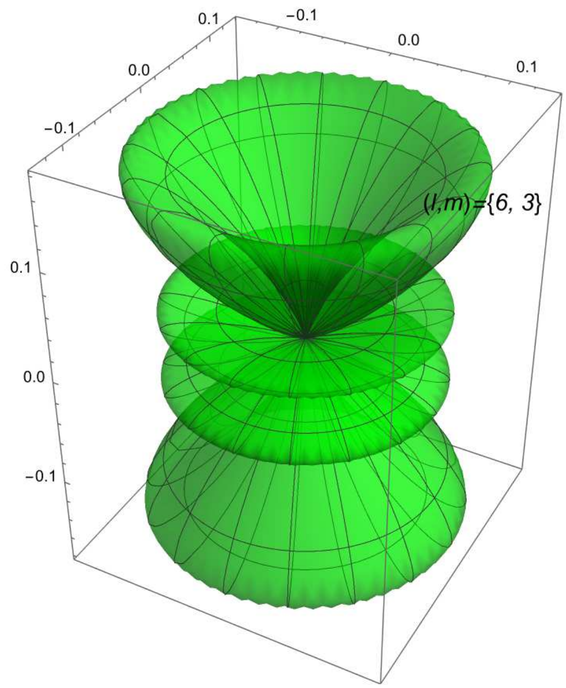

**$l$ = 6, $m$ = 6, 5, 4, 3, 2, 1, 0: SphericalPlot3D**

**Fig.14**

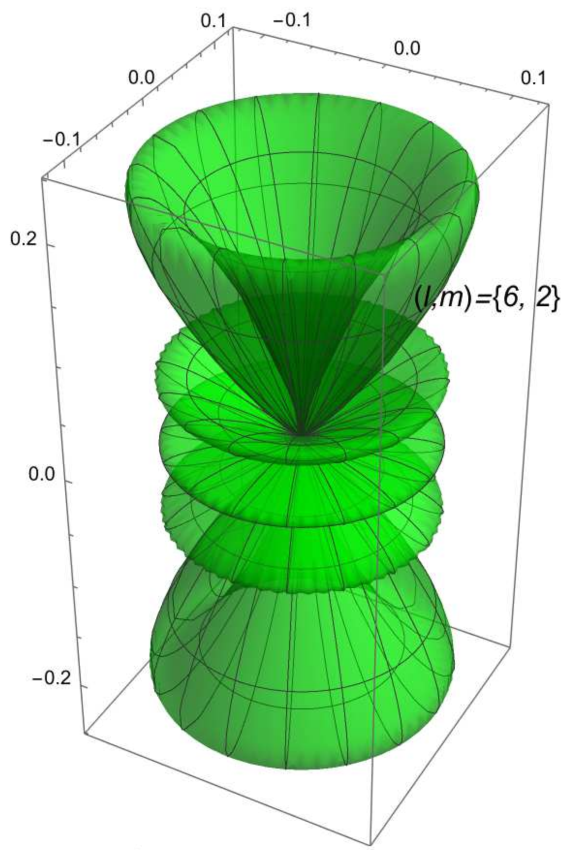

(l,m)={6, 6}
0.10
0.05
0.00
−0.2
−0.1
0.0
0.1
0.2
0.2
0.1
0.0
−0.1
−0.2


(l,m)={6, 5}
0.10
0.05
0.00
−0.05
−0.1
0.0
0.1
0.1
0.0
−0.1

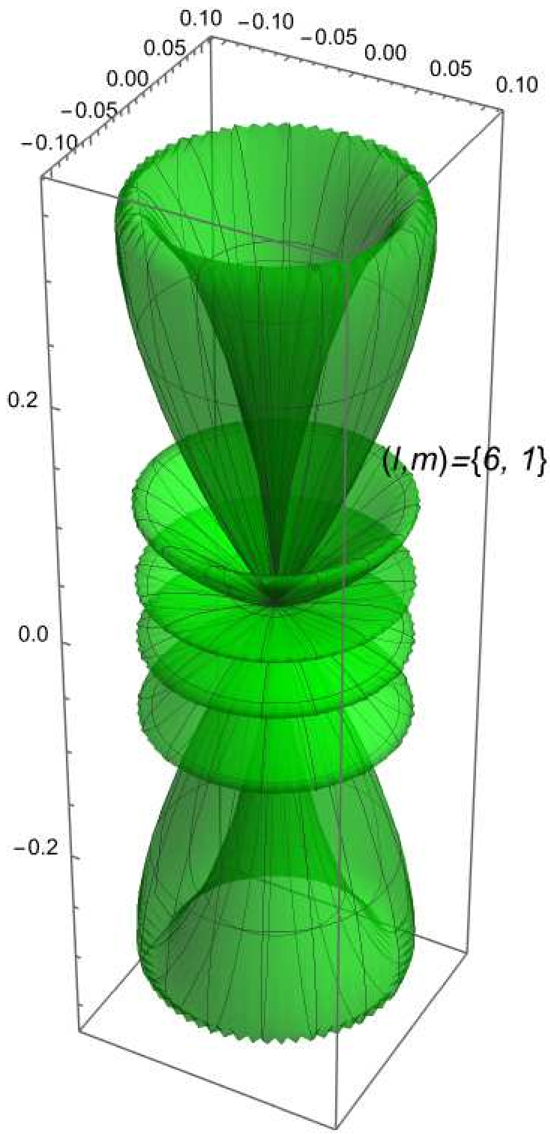

(l,m)={6, 4}
0.1
0.0
−0.1
0.1
0.0
−0.1
−0.1
0.0
0.1



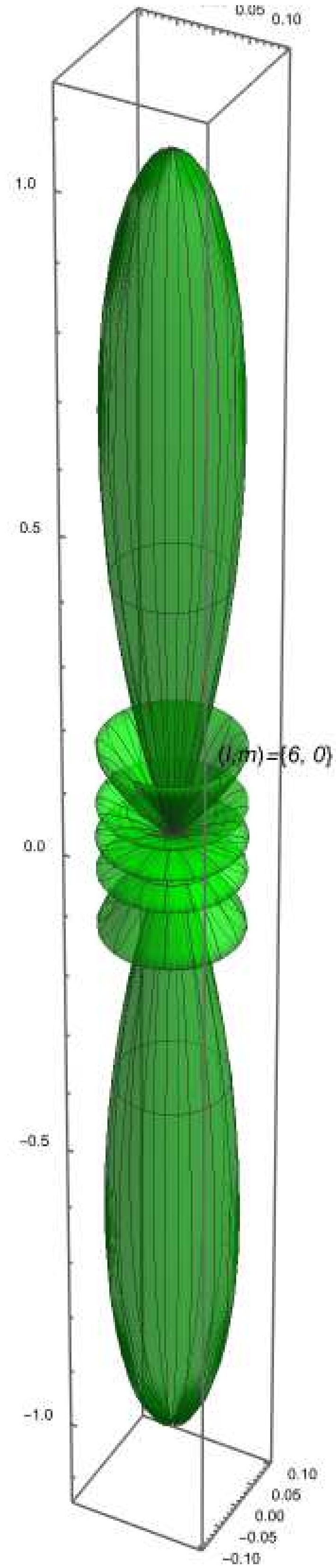
0.1
−0.1
0.0
0.1
0.0
−0.1
(l,m)={6, 3}
0.1
0.0
−0.1

0.1
−0.1
0.0
0.1
0.0
−0.1
0.2
(l,m)={6, 2}
0.0
−0.2



0.10
0.05
0.00
−0.05
−0.10
−0.10
−0.05
0.00
0.05
0.10
0.2
0.0
−0.2
$(l,m)=\{6, 1\}$



0.05 0.10
1.0
0.5
(l,m)={6, 0}
0.0
−0.5
−1.0
0.10
0.05
0.00
−0.05
−0.10

## 11. Contour plot of $\mathrm{Re}[Y_l^m(\theta,\phi)]$ on the Bloch sphere

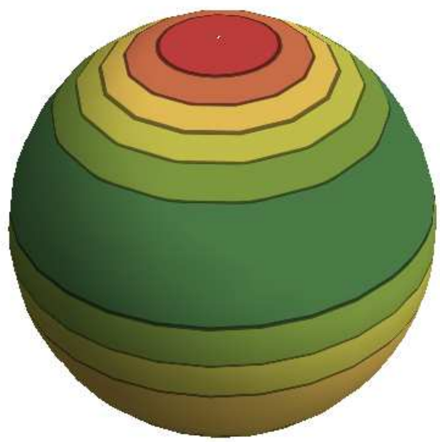
Here we show a contour plot of $\mathrm{Re}[Y_l^m(\theta,\phi)]$ for several spherical harmonics, where the contours of $\mathrm{Re}[Y_l^m(\theta,\phi)]$=constant are drawn on the unit sphere (the Bloch sphere). Since the spherical harmonics are functions on the unit sphere, the figures show a series of balls with contours drawn on them. We show the plot contours on which the squares of the real part of the spherical harmonics is constant. The contours on which $\mathrm{Re}[Y_l^m(\theta,\phi)]>0$ are denoted by red lines, while the contours on which $\mathrm{Re}[Y_l^m(\theta,\phi)]<0$ are denoted by blue lines. For large *l*, $\mathrm{Re}[Y_l^l(\theta,\phi)]$ is significantly non-zero only where $\sin\theta\approx 1$, i.e., around the equator. As *m* decreases from *m* = *l* to *m* = 0, the region of the unit sphere in which $\mathrm{Re}[Y_l^l(\theta,\phi)]$ is significantly non-zero gradually spreads from the equator towards the poles. For large *l* the phase of $\mathrm{Re}[Y_l^l(\theta,\phi)]$ changes rapidly with $\phi$. As *m* decreases, the change of the phase of $\mathrm{Re}[Y_l^l(\theta,\phi)]$ becomes smaller.

**((Mathematica-4))**

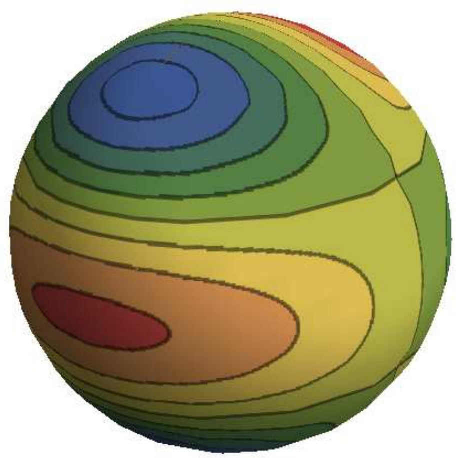
```
Clear["Global`*"];
ReYDensityPlot[ℓ_Integer, m_Integer] :=
 Block[{ymap, θ, ϕ},
  ymap =
   Image[ContourPlot[
     Re[SphericalHarmonicY[ℓ, m, θ, ϕ]] // Evaluate,
     {ϕ, 0, 2 π}, {θ, 0, π}, AspectRatio → Automatic,
     ColorFunction → "Rainbow", Frame → False,
     ImagePadding → None, PerformanceGoal → "Quality",
     PlotPoints → 80, PlotRange → All,
     PlotRangePadding → None], ImageResolution → 200];
  ParametricPlot3D[
   {Cos[ϕ] Sin[θ], Sin[ϕ] Sin[θ], Cos[θ]},
   {ϕ, 0, 2 π}, {θ, 0, π}, Lighting → "Neutral",
   Mesh → None, PlotStyle → Texture[ymap],
   Axes → False, Boxed → False,
   TextureCoordinateFunction → ({#4, #5} &)]]
```

**(i)** $\left|l=3, m\right\rangle$ state

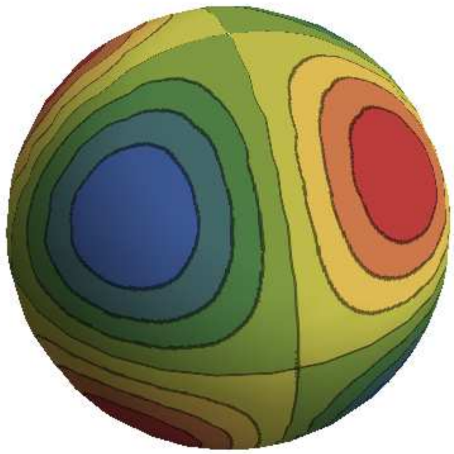
**(a)** $l = 3$, $m = 0$



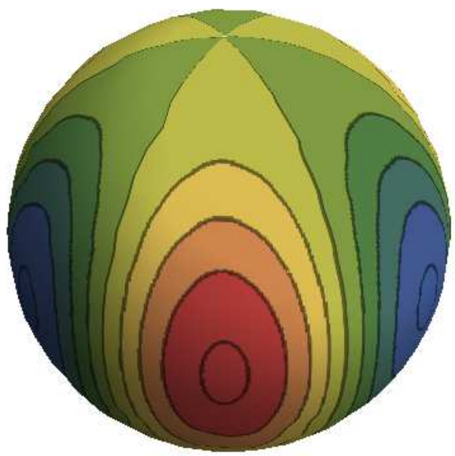
**(b)** $l = 3$, $m = 1$



**(c)** $l = 3$, $m = 2$

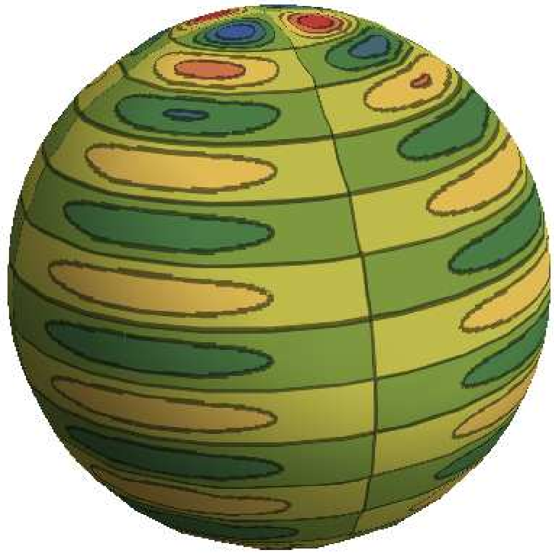


**(d)** $l = 3$, $m = 3$

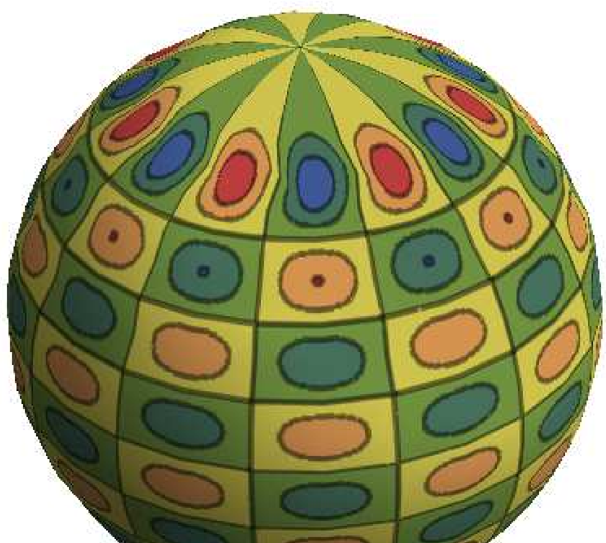


**(ii)** $\left| l = 15, m \right\rangle$ state

**(a)** $l = 15$, $m = 2$



**(b)** $l = 15, m = 7$



**(c)** $l = 15, m = 15$

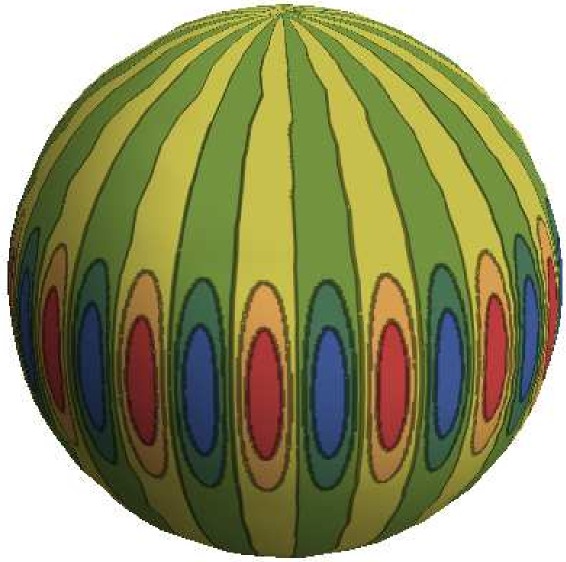


**Fig.15** Contour plot of $\mathrm{Re}[Y_l^m(\theta,\phi)]$ on the Bloch sphere

## 12. Rotational motion

We define the unit: Kaiser (cm$^{-1}$) as

$$E = \hbar\omega = \hbar ck = \frac{2\pi\hbar c}{\lambda} = \frac{1.23984\times 10^{-4}}{\lambda(cm)}[eV]$$

This is the relation between energy (erg) and Kaiser (cm$^{-1}$). When one discusses the optical spectrum, the unit (Kaiser, cm$^{-1}$) is conventionally use.

The Hamiltonian for the rotation is given by

$$\hat{H} = \frac{\hat{L}_x^{\,2}}{2I_x} + \frac{\hat{L}_z^{\,2}}{2I_y} + \frac{\hat{L}_z^{\,2}}{2I_z}$$

where $I_x$, $I_y$, and $I_z$ are the moment of inertia.

**(a)** $I_x = I_y = I_z = I$ (isotropic)

$$\hat{H} = \frac{\hat{\mathbf{L}}^2}{2I}.$$

$|l,m\rangle$ is the eigenket of $\hat{\mathbf{L}}^2$ \ with the eigenvalue $\hbar^2 l(l+1)$;

$$\hat{\mathbf{L}}^2|l,m\rangle = \hbar^2 l(l+1)|l,m\rangle .$$

Then we have

$$\hat{H}|l,m\rangle = \frac{\hbar^2 l(l+1)}{2I}|l,m\rangle = E(l)|l,m\rangle .$$

where $m = l$, $l$-1,...., -$l$+1, and -$l$. The energy level is given by

$$E(l) = \frac{\hbar^2 l(l+1)}{2I} .$$

The degeneracy of the energy level is (2$l$ + 1). Note that

$$E(l+1) - E(l) = \frac{\hbar^2 (l+1)(l+2)}{2I} - \frac{\hbar^2 l(l+1)}{2I} = \frac{\hbar^2}{I}(l+1) .$$

The wave function is given by

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

**(b)** $I_x = I_y$, but $I_z \neq I_x$

$$\hat{H} = \frac{\hat{L}_x^{\ 2} + \hat{L}_z^{\ 2}}{2I_x} + \frac{\hat{L}_z^{\ 2}}{2I_z} = \frac{\hat{\mathbf{L}}^2 - \hat{L}_z^{\ 2}}{2I_x} + \frac{\hat{L}_z^{\ 2}}{2I_z} .$$

Since $[\hat{\mathbf{L}}^2, \hat{L}_z] = 0$, $|l,m\rangle$ is the simultaneous eigenket of $\hat{\mathbf{L}}^2$ and $\hat{L}_z$ with the eigenvalue $\hbar^2 l(l+1)$ and $\hbar m$, respectively.

$$\hat{\mathbf{L}}^2|l,m\rangle = \hbar^2 l(l+1)|l,m\rangle , \qquad \hat{L}_z|l,m\rangle = \hbar m|l,m\rangle .$$

Then we have

$$\hat{H}|l,m\rangle = E(l,m)|l,m\rangle$$

where

$$E(l,m) = \frac{\hbar^2[l(l+1) - m^2]}{2I_x} + \frac{\hbar^2 m^2}{2I_z}$$

We note that

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

## 13. 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,

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

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

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

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

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

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

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

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

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

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

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

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

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

**((Mathematica-5)) Spherical harmonics using the Cartesian co-ordinate (*x*, *y*, *z*)**

## Spherical Harmonics: representation in Cartesian co-ordinates

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

$$\text{rule1} = \left\{r \to \sqrt{x^2 + y^2 + z^2},\ \theta \to \text{ArcCos}\left[\frac{z}{\sqrt{x^2 + y^2 + z^2}}\right],\ \phi \to \text{ArcTan}\left[\frac{y}{x}\right]\right\};$$

```
f[n_, m_] := Module[{g1, g2},
   g1 = r^n SphericalHarmonicY[n, m, θ, ϕ];
   g1 //. rule1 // FullSimplify[#, {x > 0, y > 0, z > 0}] &];

G[n1_] := Table[{n1, m1, f[n1, m1]}, {m1, -n1, n1, 1}] //
   TableForm;
```

l=0 (s), m = 0; even parity

```
G[0]
```

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

## l=1 (p), m = -1,0,1; odd parity

```
G[1]
```

| | | |
|---|---|---|
| 1 | -1 | $\frac{1}{2}\sqrt{\frac{3}{2\pi}}\,(x - i\,y)$ |
| 1 | 0 | $\frac{1}{2}\sqrt{\frac{3}{\pi}}\,z$ |
| 1 | 1 | $-\frac{1}{2}\sqrt{\frac{3}{2\pi}}\,(x + i\,y)$ |

l=2(d), m = -2, -1, 0, 1, 2; even parity

**G[2]**

| | | |
|---|---|---|
| 2 | -2 | $\frac{1}{4}\sqrt{\frac{15}{2\pi}}\,(x - i\,y)^2$ |
| 2 | -1 | $\frac{1}{2}\sqrt{\frac{15}{2\pi}}\,(x - i\,y)\,z$ |
| 2 | 0 | $-\frac{1}{4}\sqrt{\frac{5}{\pi}}\,(x^2 + y^2 - 2\,z^2)$ |
| 2 | 1 | $-\frac{1}{2}\sqrt{\frac{15}{2\pi}}\,(x + i\,y)\,z$ |
| 2 | 2 | $\frac{1}{4}\sqrt{\frac{15}{2\pi}}\,(x + i\,y)^2$ |

l=3 (f), m = -3, -2, -1, 0, 1, 2, 3: odd parity

G[3]

| | | |
|---|---|---|
| 3 | -3 | $\frac{1}{8}\sqrt{\frac{35}{\pi}}\,(x - i\,y)^3$ |
| 3 | -2 | $\frac{1}{4}\sqrt{\frac{105}{2\pi}}\,(x - i\,y)^2\,z$ |
| 3 | -1 | $-\frac{1}{8}\sqrt{\frac{21}{\pi}}\,(x - i\,y)\,\left(x^2 + y^2 - 4\,z^2\right)$ |
| 3 | 0 | $\frac{1}{4}\sqrt{\frac{7}{\pi}}\,z\,\left(-3\,\left(x^2 + y^2\right) + 2\,z^2\right)$ |
| 3 | 1 | $\frac{1}{8}\sqrt{\frac{21}{\pi}}\,(x + i\,y)\,\left(x^2 + y^2 - 4\,z^2\right)$ |
| 3 | 2 | $\frac{1}{4}\sqrt{\frac{105}{2\pi}}\,(x + i\,y)^2\,z$ |
| 3 | 3 | $-\frac{1}{8}\sqrt{\frac{35}{\pi}}\,(x + i\,y)^3$ |

l=4(g), m = -4, -3, -2, -1, 0, 1, 2, 3, 4; even parity

G[4]

| | | |
|---|---|---|
| 4 | -4 | $\frac{3}{16}\sqrt{\frac{35}{2\pi}}\,(x - i\,y)^4$ |
| 4 | -3 | $\frac{3}{8}\sqrt{\frac{35}{\pi}}\,(x - i\,y)^3\,z$ |
| 4 | -2 | $-\frac{3}{8}\sqrt{\frac{5}{2\pi}}\,(x - i\,y)^2\,(x^2 + y^2 - 6\,z^2)$ |
| 4 | -1 | $-\frac{3}{8}\sqrt{\frac{5}{\pi}}\,(x - i\,y)\,z\,(3\,(x^2 + y^2) - 4\,z^2)$ |
| 4 | 0 | $\frac{9\,(x^2+y^2)^2-72\,(x^2+y^2)\,z^2+24\,z^4}{16\sqrt{\pi}}$ |
| 4 | 1 | $\frac{3}{8}\sqrt{\frac{5}{\pi}}\,(x + i\,y)\,z\,(3\,(x^2 + y^2) - 4\,z^2)$ |
| 4 | 2 | $-\frac{3}{8}\sqrt{\frac{5}{2\pi}}\,(x + i\,y)^2\,(x^2 + y^2 - 6\,z^2)$ |
| 4 | 3 | $-\frac{3}{8}\sqrt{\frac{35}{\pi}}\,(x + i\,y)^3\,z$ |
| 4 | 4 | $\frac{3}{16}\sqrt{\frac{35}{2\pi}}\,(x + i\,y)^4$ |

## 14. Example-1

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

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

(a) Is $\psi(\boldsymbol{r})$ 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

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

So we get

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

with $l = 1$.

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

which is independent of $m$.

## 15. 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

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

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

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

## 16. The Series expansion of the Legendre differential equation

We note that

$$[\hat{\pi}, \hat{\boldsymbol{L}}] = 0, \text{ and } [\hat{\pi}, \hat{\boldsymbol{L}}^2] = 0,$$

where $\hat{\pi}$ is the parity operator and $\hat{\boldsymbol{L}}$ is the orbital angular momentum. Then we have a simultaneous eigenket of $\hat{\pi}$ and $\hat{\boldsymbol{L}}^2$ such that

$$\hat{\pi}|l,m\rangle = \pm|l.m\rangle, \; \hat{\boldsymbol{L}}^2|l,m\rangle = \hbar^2 l(l+1)|\psi\rangle.$$

We obtain

$$\langle\theta,\phi|\hat{\pi}|l,m\rangle = \langle\pi-\theta,\pi+\phi|\hat{\pi}|l,m\rangle = \pm\langle\theta,\phi|l,m\rangle.$$

This means that under the parity operation, we get

$$x = \cos\theta \rightarrow \cos(\pi-\theta) = -\cos\theta = -x,$$

Here we consider the case of $m = 0$. The function $y(x)$ is defined as

$$y(x) = \langle\theta,\varphi|l,m=0\rangle,$$

where

$$x = \cos\theta.$$

The function $y(x)$ is either even or odd function of $x$,

$$y(-x) = \pm y(-x).$$

depending on the value of $l$. The function $y(x)$ satisfies the differential equation

$$(1-x^2)y''(x) - 2xy'(x) + \lambda y(x) = 0.$$

where $\lambda$ is the eigenvalue to be determined. So it is reasonable to assume that

$$y(x) = x^p \sum_{k=0}^{\infty} a(2k)x^{2k} = \sum_{k=0}^{\infty} a(2k)x^{2k+p} ,$$

where $a(0) \neq 0$ and the index $p$ is expected to be either 0 (even function) or 1 (odd function). We solve the second order differential equation by using the series expansion. Then we have

$$p(p-1)a(0) = 0 ,$$

$$[\lambda - p(p+1)]a(0) + (p+1)(p+2)a(2) = 0 ,$$

$$[\lambda - (p+2)(p+3)]a(2) + (p+3)(p+4)a(4) = 0 ,$$

$$[\lambda - (p+4)(p+5)]a(4) + (p+5)(p+6)a(6) = 0 ,$$

$$[\lambda - (p+6)(p+7)]a(6) + (p+7)(p+8)a(8) = 0 ,$$

$$[\lambda - (p+8)(p+9)]a(8) + (p+9)(p+10)a(10) = 0 ,$$

……………………………………………………………

From the first equation, we have

$$p = 0 \text{, or} \qquad p = 1 .$$

In general, we have the recursion relation

$$a(2k+2) = \frac{(2k+p)(2k+p+1) - \lambda}{(2k+p+1)(2k+p+2)} a(2k)$$

When

$$\lambda = (2k+p)(2k+p+1) ,$$

we have

$$a(2k+2) = a(2k+4) = ... = 0$$

Then the series terminates. The solution is just the Legendre polynomial.

(i) $p = 0$

We have

$$a(2k+2) = \frac{(2k)(2k+1) - \lambda}{(2k+1)(2k+2)} a(2k)$$

with

$$\lambda a(0) + 2a(2) = 0$$

$$(\lambda - 6)a(2) + 12a(4) = 0$$

$$(\lambda - 20)a(4) + 30a(6) = 0$$

$$(\lambda - 42)a(6) + 56a(8) = 0$$

$$(\lambda - 72)a(8) + 90a(10) = 0$$

(ii) $p = 1$

$$a(2k+2) = \frac{(2k+1)(2k+2) - \lambda}{(2k+2)(2k+3)} a(2k)$$

with

$$(\lambda - 2)a(0) + 6a(2) = 0$$

$$(\lambda - 12)a(2) + 20a(4) = 0$$

$$(\lambda - 30)a(4) + 42a(6) = 0$$

$$(\lambda - 56)a(6) + 72a(8) = 0$$

$$(\lambda - 90)a(8) + 110a(10) = 0$$

where

$$\lambda = l(l+1)$$

**((Mathematica-6))** **Series expansion method**

```
Clear["Global`*"];
eq1 = (1 - ξ^2) D[φ[ξ], {ξ, 2}] - 2 ξ D[φ[ξ], ξ] + L (L + 1) φ[ξ];
DSolve[eq1 == 0, φ[ξ], ξ] // Simplify

{{φ[ξ] → C[1] LegendreP[L, ξ] + C[2] LegendreQ[L, ξ]}}

eq2 = (1 - ξ^2) D[φ[ξ], {ξ, 2}] - 2 ξ D[φ[ξ], ξ] + λ φ[ξ];

f1[x_] := x^p Sum[a[2 k] x^(2 k), {k, 0, 6}]; rule1 = {φ → (f1[#] &)};

eq3 = ξ^(2-p) eq2 /. rule1 // Simplify;
list1 = Table[{n, Coefficient[eq3, ξ, 2 n]}, {n, 0, 5}] //
  FullSimplify;

f2[x_] := x^p Sum[a[2 k + 2 m] x^(2 k+2 m), {m, -3, 3}];

rule2 = {φ → (f2[#] &)};

eq4 = ξ^(8-p-2 k) (eq2 /. rule2) // FullSimplify;

list2 = Table[{n, Coefficient[eq4, ξ, 2 n]}, {n, 2, 6}] //
   Simplify;

seq1 = list2[[3, 2]] == 0;

seq11 = Solve[seq1, a[2 + 2 k]] // FullSimplify;
```

```
seq12 = seq11 /. p → 1
```

$$\left\{\left\{a[2+2k] \to \frac{\left(2+6k+4k^2-\lambda\right) a[2k]}{(2+2k)(3+2k)}\right\}\right\}$$

```
seq13 = seq12 /. p → 0
```

$$\left\{\left\{a[2+2k] \to \frac{\left(2+6k+4k^2-\lambda\right) a[2k]}{(2+2k)(3+2k)}\right\}\right\}$$

```
list1 /. p → 0 // TableForm
```

| | |
|---|---|
| 0 | 0 |
| 1 | $\lambda a[0] + 2 a[2]$ |
| 2 | $-(6-\lambda) a[2] + 12 a[4]$ |
| 3 | $-(20-\lambda) a[4] + 30 a[6]$ |
| 4 | $-(42-\lambda) a[6] + 56 a[8]$ |
| 5 | $-(72-\lambda) a[8] + 90 a[10]$ |

```
list1 /. p → 1 // TableForm
```

| | |
|---|---|
| 0 | 0 |
| 1 | $-(2-\lambda) a[0] + 6 a[2]$ |
| 2 | $-(12-\lambda) a[2] + 20 a[4]$ |
| 3 | $-(30-\lambda) a[4] + 42 a[6]$ |
| 4 | $-(56-\lambda) a[6] + 72 a[8]$ |
| 5 | $-(90-\lambda) a[8] + 110 a[10]$ |

**(b) Legendre function determined from the series expansion**

(1) $l = 0$

$\lambda = 0$, $a(2) = 0$

$P_0(\xi) = a(0)$

(2) $l = 1$

$\lambda = 2$, $a(2) = 0$

$P_1(\xi) = a(0)\xi$

(3) $l = 2$

$\lambda = 6$, $a(4) = 0$, $a(2) = -3a(0)$

$P_2(\xi) = -a(0)(-1+3\xi^2)$

(4) $l = 3$

$\lambda = 12$, $a(4) = 0$, $a(2) = -\frac{5}{3}a(0)$

$P_3(\xi) = a(0)\xi(1-\frac{5}{3}\xi^2) = -\frac{a(0)}{3}(-3\xi+5\xi^3)$

(5) $l = 4$

$\lambda = 20$, $a(6) = 0$, $a(2) = -10a(0)$, $a(4) = \frac{35}{3}a(0)$

$P_4(\xi) = a(0)(1-10\xi^2+\frac{35}{3}\xi^4) = \frac{a(0)}{3}[3-30\xi^2+35\xi^4]$

Note that the value of $a(0)$ can be determined from the normalization such that

$$\int_{-1}^{1} d\mu P_l(\mu)P_{l'}(\mu) = \delta_{l,l'}\frac{2}{2l+1}$$

**(c). Legendre function (Mathematica)**

((**Mathematica**))

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

Table[{L, LegendreP[L, ξ]}, {L, 0, 10}] // TableForm
```

| | |
|---|---|
| 0 | $1$ |
| 1 | $\xi$ |
| 2 | $\frac{1}{2}\left(-1+3\,\xi^2\right)$ |
| 3 | $\frac{1}{2}\left(-3\,\xi+5\,\xi^3\right)$ |
| 4 | $\frac{1}{8}\left(3-30\,\xi^2+35\,\xi^4\right)$ |
| 5 | $\frac{1}{8}\left(15\,\xi-70\,\xi^3+63\,\xi^5\right)$ |
| 6 | $\frac{1}{16}\left(-5+105\,\xi^2-315\,\xi^4+231\,\xi^6\right)$ |
| 7 | $\frac{1}{16}\left(-35\,\xi+315\,\xi^3-693\,\xi^5+429\,\xi^7\right)$ |
| 8 | $\frac{1}{128}\left(35-1260\,\xi^2+6930\,\xi^4-12\,012\,\xi^6+6435\,\xi^8\right)$ |
| 9 | $\frac{1}{128}\left(315\,\xi-4620\,\xi^3+18\,018\,\xi^5-25\,740\,\xi^7+12\,155\,\xi^9\right)$ |
| 10 | $\frac{1}{256}\left(-63+3465\,\xi^2-30\,030\,\xi^4+90\,090\,\xi^6-109\,395\,\xi^8+46\,189\,\xi^{10}\right)$ |

---

**REFERENCE**

A.R. Edmonds, *Angular Momentum in Quantum Mechanics* (Princeton University, 1957).
M.E. Rose, *Elementary Theory of Angular Momentum* (Dover, 1995).
J. Binney and D. Skinner, *The Physics of Quantum Mechanics* (Oxford, 2014).
E. Merzbacher, *Quantum Mechanics*, 3rd edition (John Wiley & Sons, New York, 1998).
A. Goswami, Quantum Mechanics, 2nd edition (Waveland Press, 2003).
D.H. McIntyre, *Quantum Mechanics A Paradigms Approach* (Pearson Education, 2012).

## APPENDIX: Recursion formula

$$\hat{L}_+ = \hat{L}_x + i\hat{L}_y, \qquad \hat{L}_- = \hat{L}_x - i\hat{L}_y.$$

$$\hat{L}_+\left|l,m\right\rangle = \hbar\sqrt{(l-m)(l+m+1)}\left|l,m+1\right\rangle.$$

$$\hat{L}_-\left|l,m\right\rangle = \hbar\sqrt{(l+m)(l-m+1)}\left|l,m-1\right\rangle.$$

### (a) Method-I: the use of $\hat{L}_+$

Suppose that $\langle \mathbf{n}|l,m=l\rangle$ is given exactly. We determine the exact form of $\langle \mathbf{n}|l,m\rangle$ in the following way.

$$\hat{L}_+ \left| l,0 \right\rangle = \hbar\sqrt{l(l+1)}\left| l,1 \right\rangle$$

$$\hat{L}_+ \left| l,1 \right\rangle = \hbar\sqrt{(l-1)(l+2)}\left| l,2 \right\rangle$$

$$\hat{L}_+ \left| l,2 \right\rangle = \hbar\sqrt{(l-2)(l+3)}\left| l,3 \right\rangle$$

.............................................................................

$$\hat{L}_+ \left| l,m-2 \right\rangle = \hbar\sqrt{(l-m+2)(l+m-1)}\left| l,m-1 \right\rangle$$

$$\hat{L}_+ \left| l,m-1 \right\rangle = \hbar\sqrt{(l-m+1)(l+m)}\left| l,m \right\rangle$$

By multiplying terms of both sides separately, we have

$$(\hat{L}_+)^m \left| l,0 \right\rangle = \hbar^m \sqrt{l(l-1)....(l-m+1)} \\ \times\sqrt{(l+1)(l+2)....(l+m)}\left| l,m \right\rangle$$

or

$$\left| l,m \right\rangle = \frac{1}{\hbar^m}\sqrt{\frac{(l+m)!}{(l-m)!}}(\hat{L}_+)^m \left| l,0 \right\rangle$$

or

$$\left\langle \mathbf{n} \middle| l,m \right\rangle = \frac{1}{\hbar^m}\sqrt{\frac{(l+m)!}{(l-m)!}}(L_+)^m \left\langle \mathbf{n} \middle| l,0 \right\rangle$$

where $L_+$ is the differential operator and is given by

$$L_+ = \hbar e^{i\phi}(\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\phi})$$

In Mathematica, this differential operator is given by

$$L_+ \to \hbar e^{i\phi}(D[\#,\theta] + +i\cot\theta D[\#,\phi])\ \&$$

**(b) Method-II: the use of $\hat{L}_-$**

Suppose that $\langle \mathbf{n} | l, m = l \rangle$ is given exactly. We determine the exact form of $\langle \mathbf{n} | l, m \rangle$ in the following way.

$$\hat{L}_- | l, l \rangle = \hbar \sqrt{2l \cdot 1} | l, l-1 \rangle ,$$

$$\hat{L}_- | l, l-1 \rangle = \hbar \sqrt{(2l-1) \cdot 2} | l, l-2 \rangle ,$$

$$\hat{L}_- | l, l-2 \rangle = \hbar \sqrt{(2l-2) \cdot 3} | l, l-3 \rangle$$

……………………………………………………………………………….

$$\hat{L}_- | l, m+2 \rangle = \hbar \sqrt{(l+m+2)(l-m-1)} | l, m+1 \rangle$$

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

By multiplying these terms of both sides separately, we have

$$(\hat{L}_-)^{l-m} | l, l \rangle = \hbar^{l-m} \sqrt{\frac{(2l)!(l-m)!}{(l+m)!}} | l, m \rangle$$

or

$$| l, m \rangle = \frac{1}{\hbar^{l-m}} \sqrt{\frac{(l+m)!}{(2l)!(l-m)!}} (\hat{L}_-)^{l-m} | l, l \rangle$$

or

$$\langle \mathbf{n} | l, m \rangle = \frac{1}{\hbar^{l-m}} \sqrt{\frac{(l+m)!}{(2l)!(l-m)!}} (L_-)^{l-m} \langle \mathbf{n} | l, l \rangle$$

where $L_+$ is the differential operator

$$L_- = \hbar e^{-i\phi} (-\frac{\partial}{\partial \theta} + i \cot\theta \frac{\partial}{\partial \phi})$$

In Mathematics, the differential operator is given by

$$L_- \to \hbar e^{-i\phi}(-D[\#,\theta]+i\cot\theta D[\#,\phi])\,\&$$

((**Note**))

$$L_+ = \hbar e^{i\phi}(\frac{\partial}{\partial\theta}+i\cot\theta\frac{\partial}{\partial\phi}),$$

$$L_- = \hbar e^{-i\phi}(-\frac{\partial}{\partial\theta}+i\cot\theta\frac{\partial}{\partial\phi}),$$

with

$$L_x = i\hbar(\sin\phi\frac{\partial}{\partial\theta}+\cot\theta\cos\phi\frac{\partial}{\partial\phi}).$$

$$L_y = i\hbar(-\cos\phi\frac{\partial}{\partial\theta}+\cot\theta\sin\phi\frac{\partial}{\partial\phi}).$$

$$L_z = -i\hbar\frac{\partial}{\partial\phi}.$$

(**a**)

Differential operator:

$$L_+^{\ *} = \hbar e^{-i\phi}(\frac{\partial}{\partial\theta}-i\cot\theta\frac{\partial}{\partial\phi}) = -L_-.$$

For the operators in quantum mechanics

$$\hat{L}_+^{\ +} = \hat{L}_x - i\hat{L}_y = \hat{L}_-, \qquad \hat{L}_-^{\ +} = \hat{L}_x + i\hat{L}_y = \hat{L}_+.$$

$$\begin{aligned}\langle \mathbf{n}|\hat{L}_+|\psi\rangle &= \langle \psi|\hat{L}_+{}^+|\mathbf{n}\rangle^* \\ &= \langle \psi|\hat{L}_-|\mathbf{n}\rangle^* \\ &= [-L_-\langle \psi|\mathbf{n}\rangle]^* \\ &= -L_-^*\langle \psi|\mathbf{n}\rangle^* \\ &= L_+\langle \mathbf{n}|\psi\rangle\end{aligned}$$

$$\begin{aligned}\langle \mathbf{n}|\hat{L}_-|\psi\rangle &= \langle \psi|\hat{L}_-{}^+|\mathbf{n}\rangle^* \\ &= \langle \psi|\hat{L}_+|\mathbf{n}\rangle^* \\ &= [-L_+\langle \psi|\mathbf{n}\rangle]^* \\ &= -L_+^*\langle \psi|\mathbf{n}\rangle^* \\ &= L_-\langle \mathbf{n}|\psi\rangle\end{aligned}$$

Note that

$$\langle \psi|\hat{L}_+{}^+|\mathbf{n}\rangle = -L_-\langle \psi|\mathbf{n}\rangle,$$

$$\langle \psi|\hat{L}_-{}^+|\mathbf{n}\rangle = -L_+\langle \psi|\mathbf{n}\rangle.$$

**(b)**

$$\begin{aligned}\langle \psi|\hat{L}_+{}^+|\mathbf{n}\rangle &= \langle \psi|\hat{L}_-|\mathbf{n}\rangle \\ &= \langle \mathbf{n}|\hat{L}_+|\psi\rangle^* \\ &= [\hbar e^{i\phi}(\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\phi})\psi(\mathbf{n})]^* \\ &= \hbar e^{-i\phi}(\frac{\partial}{\partial\theta} - i\cot\theta\frac{\partial}{\partial\phi})\psi^*(\mathbf{n}) \\ &= -L_-\psi^*(\mathbf{n}) \\ &= -L_-\langle \psi|\mathbf{n}\rangle\end{aligned}$$

$$
\begin{aligned}
\langle\psi|\hat{L}_-{}^+|\mathbf{n}\rangle &= \langle\psi|\hat{L}_+|\mathbf{n}\rangle \\
&= \langle\mathbf{n}|\hat{L}_-|\psi\rangle^* \\
&= [\hbar e^{-i\phi}(-\frac{\partial}{\partial\theta}+i\cot\theta\frac{\partial}{\partial\phi})\psi(\mathbf{n})]^* \\
&= \hbar e^{i\phi}(-\frac{\partial}{\partial\theta}-i\cot\theta\frac{\partial}{\partial\phi})\psi^*(\mathbf{n}) \\
&= -L_+\psi^*(\mathbf{n}) \\
&= -L_+\langle\psi|\mathbf{n}\rangle
\end{aligned}
$$

**((Mathematica))**

## Recursion formula for the lowering operator for spherical harmonics

### (a) Determination of spherical harmonics <n|l,m=0> from <n|l,m> using the recursion relation with rasing operator

```
Clear["Global`"];

y1[l_, θ_] := Sqrt[(2 l + 1)/(4 π)] LegendreP[l, Cos[θ]];

JR := (ⅇ^(ⅈ ϕ) (D[#, θ] + ⅈ Cot[θ] × D[#, ϕ])) &;

Y[l_, m_, θ_, ϕ_] := (Sqrt[(l - m)!/(l + m)!] Nest[JR, #, m]) &;

g1[L_] := Module[{eq1, L1, s1}, L1 = L;
  eq1 = Table[{L1, m1, Y[L1, m1, θ, ϕ][y1[L1, θ]] }, {m1, 0, L1, 1}] //
    Simplify; s1 = Prepend[eq1, {"  L  ", " M  ", " Y(L,M, θ,ϕ)   "}];
  Grid[s1]];

g1[1] // Simplify
```

| L | M | Y(L,M, θ,ϕ) |
|---|---|---|
| 1 | 0 | $\frac{1}{2}\sqrt{\frac{3}{\pi}}\,\mathrm{Cos}[\theta]$ |
| 1 | 1 | $-\frac{1}{2}e^{i\phi}\sqrt{\frac{3}{2\pi}}\,\mathrm{Sin}[\theta]$ |

```
g1[2] // Simplify
```

| L | M | Y(L,M, θ,ϕ) |
|---|---|---|
| 2 | 0 | $\frac{1}{8}\sqrt{\frac{5}{\pi}}\,(1+3\,\text{Cos}[2\,\theta])$ |
| 2 | 1 | $-\frac{1}{2}\,e^{i\,\phi}\sqrt{\frac{15}{2\,\pi}}\,\text{Cos}[\theta]\times\text{Sin}[\theta]$ |
| 2 | 2 | $\frac{1}{4}\,e^{2\,i\,\phi}\sqrt{\frac{15}{2\,\pi}}\,\text{Sin}[\theta]^2$ |

```
g1[3] // Simplify
```

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

```
g1[4] // Simplify
```

| L | M | Y(L,M, θ,ϕ) |
|---|---|---|
| 4 | 0 | $\frac{3\,(9+20\,\text{Cos}[2\,\theta]+35\,\text{Cos}[4\,\theta])}{128\,\sqrt{\pi}}$ |
| 4 | 1 | $-\frac{3}{32}\,e^{i\,\phi}\sqrt{\frac{5}{\pi}}\,(1+7\,\text{Cos}[2\,\theta])\,\text{Sin}[2\,\theta]$ |
| 4 | 2 | $\frac{3}{16}\,e^{2\,i\,\phi}\sqrt{\frac{5}{2\,\pi}}\,(5+7\,\text{Cos}[2\,\theta])\,\text{Sin}[\theta]^2$ |
| 4 | 3 | $-\frac{3}{8}\,e^{3\,i\,\phi}\sqrt{\frac{35}{\pi}}\,\text{Cos}[\theta]\,\text{Sin}[\theta]^3$ |
| 4 | 4 | $\frac{3}{16}\,e^{4\,i\,\phi}\sqrt{\frac{35}{2\,\pi}}\,\text{Sin}[\theta]^4$ |

## (b) Determination of spherical harmonics <n|l,m=l> from <n|l,m> using the recursion relation with lowering operator

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

$$z1[l\_,\ \theta\_,\ \phi\_] := \frac{(-1)^{l}}{2^{l}\ l\,!}\sqrt{\frac{(2\ l+1)\,!}{4\,\pi}}\ (\mathrm{Sin}[\theta])^{l}\ \mathrm{Exp}[i\ l\ \phi];$$

$$JL := \left(e^{-i\,\phi}\ (-D[\#,\ \theta] + i\,\mathrm{Cot}[\theta]\times D[\#,\ \phi])\right)\ \&;$$

$$Z[l\_,\ m\_,\ \theta\_,\ \phi\_] := \left(\sqrt{\frac{(l+m)\,!}{(2\ l)\,!\ (l-m)\,!}}\ \mathrm{Nest}[JL,\ \#,\ l-m]\right)\ \&;$$

```
h1[L_] := Module[{eq1, L1, s1}, L1 = L;
  eq1 = Table[{L1, m1, Y[L1, m1, θ, ϕ] [y1[L1, θ]] }, {m1, 0, L1, 1}] //
    Simplify; s1 = Prepend[eq1, {"  L  ", " M  ", " Y(L,M, θ,ϕ)  "}];
  Grid[s1]];
```

```
h1[1] // Simplify
```

| L | M | Y(L,M, θ,ϕ) |
|---|---|---|
| 1 | 0 | $\frac{1}{2}\sqrt{\frac{3}{\pi}}\ \mathrm{Cos}[\theta]$ |
| 1 | 1 | $-\frac{1}{2}\ e^{i\,\phi}\ \sqrt{\frac{3}{2\pi}}\ \mathrm{Sin}[\theta]$ |

```
h1[2] // Simplify
```

| L | M | Y(L,M, θ,ϕ) |
|---|---|---|
| 2 | 0 | $\frac{1}{8}\sqrt{\frac{5}{\pi}}\ (1+3\ \mathrm{Cos}[2\,\theta])$ |
| 2 | 1 | $-\frac{1}{2}\ e^{i\,\phi}\ \sqrt{\frac{15}{2\pi}}\ \mathrm{Cos}[\theta]\times\mathrm{Sin}[\theta]$ |
| 2 | 2 | $\frac{1}{4}\ e^{2\,i\,\phi}\ \sqrt{\frac{15}{2\pi}}\ \mathrm{Sin}[\theta]^{2}$ |

```
h1[3] // Simplify
```

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

```
h1[4] // Simplify
```

| L | M | $Y(L,M,\ \theta,\phi)$ |
|---|---|---|
| 4 | 0 | $\frac{3\,(9+20\,\text{Cos}[2\,\theta]+35\,\text{Cos}[4\,\theta])}{128\,\sqrt{\pi}}$ |
| 4 | 1 | $-\frac{3}{32}\,e^{i\,\phi}\sqrt{\frac{5}{\pi}}\ (1+7\,\text{Cos}[2\,\theta])\ \text{Sin}[2\,\theta]$ |
| 4 | 2 | $\frac{3}{16}\,e^{2\,i\,\phi}\sqrt{\frac{5}{2\,\pi}}\ (5+7\,\text{Cos}[2\,\theta])\ \text{Sin}[\theta]^2$ |
| 4 | 3 | $-\frac{3}{8}\,e^{3\,i\,\phi}\sqrt{\frac{35}{\pi}}\ \text{Cos}[\theta]\ \text{Sin}[\theta]^3$ |
| 4 | 4 | $\frac{3}{16}\,e^{4\,i\,\phi}\sqrt{\frac{35}{2\,\pi}}\ \text{Sin}[\theta]^4$ |