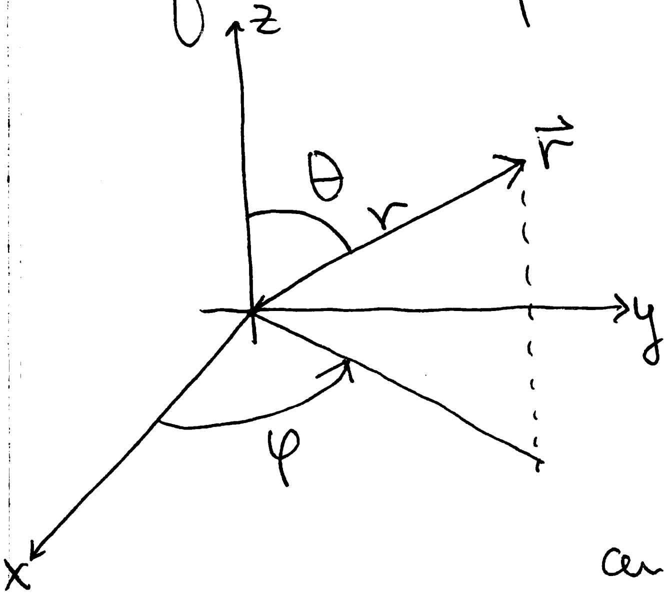
3.2. Spherical Polar Coordinates and Spherical Harmonics

In order to exploit the fact that the potential only depends upon the distance $|\vec{r}|$ we transform $\vec{r}$ to spherical polar coordinates:



$$x = r\sin\theta\cos\varphi$$
$$y = r\sin\theta\sin\varphi$$
$$z = r\cos\theta$$

$$0 \le \theta \le \pi$$
$$0 \le \varphi \le 2\pi$$

and $r^2 = x^2 + y^2 + z^2$.

The Laplacian ∇^2 in spherical polar coordinates is just

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\varphi^2} .$$

Once again, since $V = V(|\vec{r}|) = V(r)$, we try to solve the Schrödinger equation by separation of variables,

$\psi(\vec{r}) = R(r)Y(\theta,\varphi)$. Substituting into the Schrödinger equation, multiplying by r^2 and dividing by $\psi(\vec{r})$ yields

$$\overbrace{\frac{1}{R(r)}\left[\frac{-\hbar^2}{2m}\frac{d}{dr}\left(r^2\frac{d}{dr}R(r)\right) + r^2\left(V(r)-E\right)R(r)\right]}^{\text{function of } r \text{ only} = -\frac{\hbar^2}{2m}\lambda \;(=\text{separation constant})}$$

$$= \underbrace{-\frac{1}{Y(\theta,\varphi)\sin^2\theta}\left[\frac{-\hbar^2}{2m}\right]\left[\sin\theta\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}Y(\theta,\varphi)\right) + \frac{\partial^2}{\partial\varphi^2}Y(\theta,\varphi)\right]}_{\text{function of } \theta,\varphi \text{ only} = -\frac{\hbar^2}{2m}\lambda \;(=\text{separation constant})}$$

Thus we have the separated equations,

$$\boxed{\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}R(r)\right) + \left[\frac{2m}{\hbar^2}\left(E-V(r)\right) - \frac{\lambda}{r^2}\right]R(r) = 0,}$$

the radial equation, and

$$\boxed{\begin{array}{l}\text{the angular equation}\\[1em] \sin\theta\dfrac{\partial}{\partial\theta}\left(\sin\theta\dfrac{\partial}{\partial\theta}Y(\theta,\varphi)\right)+\lambda\sin^2\theta\, Y(\theta,\varphi)\\[1em] \qquad\qquad +\dfrac{\partial^2}{\partial\varphi^2}Y(\theta,\varphi)=0\end{array}}$$

Since the φ-derivative is isolated we can try separation of the angular variables

$$Y(\theta,\varphi)=A\,\Theta(\cos\theta)\,\Phi(\varphi)$$

where $A=$ constant which will be used later to normalize $Y(\theta,\varphi)$. Substituting into the angular equation and dividing by $Y(\theta,\varphi)$ yields

$$\underbrace{\frac{1}{\Theta(\cos\theta)}\left[\sin\theta\frac{d}{d\theta}\left(\sin\theta\frac{d}{d\theta}\Theta(\cos\theta)\right)+\lambda\sin^2\theta\,\Theta(\cos\theta)\right]}^{\text{function of }\theta=\nu=(\text{separation constant})}$$

$$=\underbrace{-\frac{1}{\Phi(\varphi)}\frac{d^2}{d\varphi^2}\Phi(\varphi)}_{\text{function of }\varphi\equiv\nu\,(=\text{separation constant})}$$

Thus we have the polar angular equation

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d}{d\theta}\Theta(\cos\theta)\right)$$

$$+\left(\lambda-\frac{\nu}{\sin^2\theta}\right)\Theta(\cos\theta)=0$$

and the azimuthal angle equation

$$\frac{d^2}{d\varphi^2}\Phi(\varphi)+\nu\Phi(\varphi)=0 \quad .$$

The azimuthal equation has the solutions

$$\Phi(\varphi)=\begin{cases} Ae^{i\sqrt{\nu}\varphi}+Be^{-i\sqrt{\nu}\varphi} & , \nu\neq 0 \\ A'+B'\varphi & , \nu=0 \end{cases} .$$

Since the wavefunction and its derivative, $\Phi(\varphi)$ and $\frac{d\Phi(\varphi)}{d\varphi}$, are continuous throughout the domain $0\leq\varphi\leq 2\pi$ and in particular after rotation by 2π (we require single valuedness, $\Phi(0)=\Phi(2\pi)$), $\sqrt{\nu}$ must be an integer m, $\sqrt{\nu} = m$. Further this implies that for $\nu = 0$, $B' = 0$. Thus all cases and solutions can be written as

$$\boxed{\Phi_m(\varphi) = A e^{im\varphi} \quad , \quad m = 0, \pm 1, \pm 2, \ldots}$$

* See page -182'-.

The polar angle equation with $\nu = m^2$ becomes

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta \frac{d}{d\theta}\Theta(\cos\theta)\right) + \left(\lambda - \frac{m^2}{\sin^2\theta}\right)\Theta(\cos\theta) = 0 .$$

Letting $\xi \equiv \cos\theta$ so that $\left(0 \leq \theta \leq \pi \Leftrightarrow -1 \leq \xi \leq +1\right)$

$$\frac{d}{d\theta} = \frac{d\xi}{d\theta}\frac{d}{d\xi} = -\sin\theta \frac{d}{d\xi}$$ we have

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d}{d\theta}\Theta(\cos\theta)\right)$$

$$= \frac{1}{\sin\theta}\left(-\sin\theta\frac{d}{d\xi}\right)\left(-\sin^2\theta\frac{d}{d\xi}\Theta(\xi)\right)$$

$$= \frac{d}{d\xi}\left[\sin^2\theta\frac{d}{d\xi}\Theta(\xi)\right]$$

$$= \frac{d}{d\xi}\left[(1-\xi^2)\frac{d\Theta(\xi)}{d\xi}\right] .$$

As usual we should only ask for the probability and probability current densities to be single-valued. Combining, as before, this with the principle of superposition implies that, for $\psi = \chi e^{im\varphi}$,

$$|\chi_1 e^{im_1\varphi} + \chi_2 e^{im_2\varphi}|^2 \text{ be single-valued}$$

$$= |\chi_1|^2 + |\chi_2|^2 + \chi_1^* \chi_2 e^{i(m_2-m_1)\varphi} + \chi_2^* \chi_1 e^{i(m_1-m_2)\varphi}$$

thus $m_1 - m_2 = \text{integer}$, if this is to be single-valued. Now if m is a solution, so is $-m$, since the differential equation depends on $\nu = m^2$. So we have that

$$|\chi_1 e^{im\varphi} + \chi_2 e^{-im\varphi}|^2 \text{ is single-valued}$$

$$= |\chi_1|^2 + |\chi_2|^2 + \chi_1^* \chi_2 e^{-2im\varphi} + \chi_2^* \chi_1 e^{+2im\varphi}$$

$\Rightarrow$ $2m = \text{integer}$. Thus we have two possibilities $m = 0, \pm 1, \pm 2, \ldots$ or $m = \pm\frac{1}{2}, \pm\frac{3}{2}, \ldots$,

The odd half integer set implies $\psi(2\pi) = -\psi(0)$, we cannot rule this out! Either set is acceptable, but they are exclusive either $m = 0, \pm 1, \pm 2, \ldots$ or $m = \pm\frac{1}{2}, \pm\frac{3}{2}, \ldots$ (these are complete for odd functions centered on π). Since we desire $\underline{1} = e^{i0}$ as a solution $|\chi_1 + \chi_2 e^{im\varphi}|^2$ is singlevalued $\Rightarrow m = \text{integer}$.

The polar angle equation becomes

$$\frac{d}{d\xi}\left[(1-\xi^2)\frac{d\Theta(\xi)}{d\xi}\right]+\left(\lambda-\frac{m^2}{1-\xi^2}\right)\Theta(\xi)=0.$$

The last term above is singular as $\xi\to\pm1$, the singular term, $-\frac{m^2}{1-\xi^2}\Theta(\xi)$, can be eliminated by defining

$$\Theta(\xi)\equiv(1-\xi^2)^{\frac{|m|}{2}}y(\xi).$$

We then have

$$\frac{d\Theta}{d\xi}=-|m|\xi(1-\xi^2)^{\frac{|m|}{2}-1}y+(1-\xi^2)^{|m|/2}y'$$

and hence

$$\frac{d}{d\xi}\left[(1-\xi^2)\frac{d\Theta}{d\xi}\right]=\frac{d}{d\xi}\left[-|m|\xi(1-\xi^2)^{\frac{|m|}{2}}y+(1-\xi^2)^{\frac{|m|}{2}+1}y'\right]$$

$$=\left(-|m|(1-\xi^2)^{\frac{|m|}{2}}y+m^2\xi^2(1-\xi^2)^{\frac{|m|}{2}-1}y-|m|\xi(1-\xi^2)^{\frac{|m|}{2}}y'\right)$$
$$-(|m|+2)\xi(1-\xi^2)^{\frac{|m|}{2}}y'+(1-\xi^2)^{\frac{|m|}{2}+1}y''$$

$$=\left(-|m|(1-\xi^2)+m^2\xi^2\right)(1-\xi^2)^{\frac{|m|}{2}-1}y$$
$$-2(|m|+1)\xi(1-\xi^2)^{\frac{|m|}{2}}y'+(1-\xi^2)^{\frac{|m|}{2}+1}y''$$

So the differential equation becomes, after multiplying by $(1-\xi^2)^{-\frac{|m|}{2}}$,

$$(1-\xi^2)\frac{d^2}{d\xi^2}\mathcal{J}(\xi) - 2(|m|+1)\xi\frac{d}{d\xi}\mathcal{J}(\xi) + \left(\lambda - \frac{m^2}{1-\xi^2} - |m| + \frac{m^2\xi^2}{1-\xi^2}\right)\mathcal{J}(\xi) = 0,$$

that is

$$\boxed{(1-\xi^2)\frac{d^2}{d\xi^2}\mathcal{J}(\xi) - 2(|m|+1)\xi\frac{d}{d\xi}\mathcal{J}(\xi) + \underbrace{(\lambda - m^2 - |m|)}_{=(\lambda - |m|(|m|+1))}\mathcal{J}(\xi) = 0}$$

This equation is satisfied by writing

$$\boxed{\mathcal{J}(\xi) \equiv \frac{d^{|m|}}{d\xi^{|m|}}P(\xi)}$$

with $P(\xi)$ obeying the differential equation for $m=0$,

$$\boxed{(1-\xi^2)\frac{d^2P(\xi)}{d\xi^2} - 2\xi\frac{dP(\xi)}{d\xi} + \lambda P(\xi) = 0.}$$

To establish this take the ξ-derivative $|m|$ times using the chain rule

$$\frac{d^{|m|}}{d\xi^{|m|}}\left(\xi f(\xi)\right) = \xi \frac{d^{|m|} f(\xi)}{d\xi^{|m|}} + |m| \frac{d^{|m|-1} f(\xi)}{d\xi^{|m|-1}}$$

and

$$\frac{d^{|m|}}{d\xi^{|m|}}\left[(1-\xi^2) f(\xi)\right] = (1-\xi^2)\frac{d^{|m|} f(\xi)}{d\xi^{|m|}}$$
$$+ |m|(-2\xi) \frac{d^{|m|-1} f(\xi)}{d\xi^{|m|-1}}$$
$$+ \frac{|m|(|m|-1)(-2)}{2!} \frac{d^{|m|-2} f(\xi)}{d\xi^{|m|-2}}$$

Apling these equations to the $m=0$ defining differential equation for $P(\xi)$ we have

$$\frac{d^{|m|}}{d\xi^{|m|}}\left\{(1-\xi^2)\frac{d^2 P(\xi)}{d\xi^2} - 2\xi \frac{dP(\xi)}{d\xi} + \lambda P(\xi)\right\} = 0$$

$$= \left[(1-\xi^2)\frac{d^2}{d\xi^2} \frac{d^{|m|} P(\xi)}{d\xi^{|m|}} - 2\xi |m| \frac{d}{d\xi} \frac{d^{|m|} P(\xi)}{d\xi^{|m|}} \right.$$
$$\left. - |m|(|m|-1) \frac{d^{|m|} P(\xi)}{d\xi^{|m|}}\right]$$
$$-2\xi \frac{d}{d\xi} \frac{d^{|m|} P(\xi)}{d\xi^{|m|}} - 2|m| \frac{d^{|m|} P(\xi)}{d\xi^{|m|}} + \lambda \frac{d^{|m|} P(\xi)}{d\xi^{|m|}}$$

Gathering terms we have

$$(1-\xi^2)\frac{d^2}{d\xi^2}\frac{d^{|m|}P(\xi)}{d\xi^{|m|}}$$

$$-2\xi(|m|+1)\frac{d}{d\xi}\frac{d^{|m|}P(\xi)}{d\xi^{|m|}}$$

$$+\left(\lambda-|m|(|m|+1)\right)\frac{d^{|m|}P(\xi)}{d\xi^{|m|}}=0,$$

hence $\mathcal{Z}(\xi)=\dfrac{d^{|m|}}{d\xi^{|m|}}P(\xi)$ obeys the polar angle equation. Thus we have found that, for $-1\leq\xi\leq+1$,

$$\Theta(\xi)=(1-\xi^2)^{\frac{|m|}{2}}\frac{d^{|m|}}{d\xi^{|m|}}P(\xi)$$

where $P(\xi)$ obeys the equation

$$(1-\xi^2)\frac{d^2}{d\xi^2}P(\xi)-2\xi\frac{d}{d\xi}P(\xi)+\lambda P(\xi)=0$$

that is

$$\frac{d}{d\xi}\left[(1-\xi^2)\frac{d}{d\xi}P(\xi)\right]+\lambda P(\xi)=0.$$

As we know, this is just Legendre's equation for $P(\xi)$. It has well behaved solutions in the region $-1 \le \xi \le +1$ including the endpoints $\xi = \pm 1$ only if the separation constant λ has the discrete values $\lambda = l(l+1)$, $l = 0, 1, 2, \ldots$. The resulting solutions $P_l(\xi)$ are then polynomials, the Legendre polynomials,

$$P_l(\xi) = \frac{1}{2^l l!} \frac{d^l}{d\xi^l} (\xi^2 - 1)^l \, .$$

To see this let's note a few simple properties of $P(\xi)$ that follow from the defining differential equation

1) if $P(\xi)$ is a solution to the DE then $P(-\xi)$ is also a solution. This implies that the solutions are even and odd functions of ξ

$$P(\xi) \pm P(-\xi)$$

2) if $P(\xi) \to \xi^\mu$ as $\xi \to 0$ then setting the coefficient of $\xi^{\mu-2}$ in the DE to zero implies $\mu(\mu-1) = 0$. Thus $\mu = 0$ or $\mu = 1$. This categorizes 2 classes of solutions even or odd with $P(\xi) \sim \xi^0$ or ξ^1 as $\xi \to 0$.

The above properties noted, consider the general power series solution for $P(\xi)$

$$P(\xi) = \sum_{L=0}^{\infty} a_L \xi^L , \quad \text{so}$$

$$P'(\xi) = \sum_{L=1}^{\infty} L a_L \xi^{L-1}$$

$$P''(\xi) = \sum_{L=2}^{\infty} L(L-1) a_L \xi^{L-2} .$$

The differential equation becomes

$$(1-\xi^2)P''(\xi) - 2\xi P'(\xi) + \lambda P(\xi) = 0$$

$$\Rightarrow \sum_{L=2}^{\infty} L(L-1) a_L \left(\xi^{L-2} - \xi^L\right)$$

$$- \sum_{L=1}^{\infty} 2L a_L \xi^L + \sum_{L=0}^{\infty} \lambda a_L \xi^L = 0$$

or, writing out the first couple of terms and re-labelling the summation index so that all powers of ξ are L,

$$\sum_{L=2}^{\infty} \xi^L \left[-L(L-1)a_L + (L+2)(L+1)a_{L+2} - 2La_L + \lambda a_L \right]$$

$$+ 2a_2 \xi^0 + 3\cdot 2 a_3 \xi^1 - 2a_1 \xi^1 + \lambda a_0 \xi^0$$

$$+ \lambda a_1 \xi^1 = 0$$

Thus gathering the ξ^0, ξ^1, ξ^L, $L\geq 2$ powers and setting them to zero, we find

$$\boxed{\begin{array}{l} 1)\ \lambda a_0 + 2a_2 = 0 \Rightarrow 2a_2 = -\lambda a_0 \\ 2)\ 6a_3 + \lambda a_1 - 2a_1 = 0 \Rightarrow 6a_3 = (2-\lambda)a_1 \\ 3)\ (L+1)(L+2)a_{L+2} = \underbrace{L(L-1)a_L + 2La_L - \lambda a_L}_{=[L(L+1)-\lambda]a_L} \\ \quad \text{for } L\geq 2. \end{array}}$$

Now suppose $\lambda \neq l(l+1)$, $l=0,1,2,\dots$, then

$$\frac{a_{L+2}}{a_L} = \frac{L(L+1)-\lambda}{(L+1)(L+2)} \xrightarrow{L\to\infty} 1 .$$

So as $\xi \to 1$, the series will diverge like

$$\frac{1}{(1-\xi^2)} = \sum_{L=0}^{\infty}(-1)^L(\xi^2)^L \quad \text{since this}$$

has $\dfrac{a_{L+2}}{a_L} = 1$, for all L. Then $\Theta(\xi)$

will diverge like

$$\Theta(\xi) \sim \frac{1}{(1-\xi^2)^{1+\frac{|m|}{2}}} \quad \text{as } \xi \to \pm 1 .$$

But the wavefunction ψ is to be finite over the whole domain $0 \le \theta \le \pi$, that is $-1 \le \xi \le +1$. Hence we must choose λ to be some integer given by

$$\boxed{\lambda = l(l+1) \quad , l = 0, 1, 2, 3, \ldots}$$

Then the power series for $P(\xi)$ terminates after $L = l$,

$$\frac{a_{L+2}}{a_L} = \frac{L(L+1) - l(l+1)}{(L+1)(L+2)} ,$$

So for $L \ge l$ $a_{L+2} = 0$. The $P(\xi)$ are polynomials of order l, the Legendre polynomials. Since $\Theta(\xi)$ is proportional to the $|m|^{th}$ derivative of $P(\xi)$, it vanishes unless $|m| \le l$. Hence each value of l allows $2l+1$ values of m, running from $-l$ to $+l$.

So, with $\lambda = l(l+1)$, we can solve the recursion relations

$$a_{L+2} = \frac{L(L+1) - l(l+1)}{(L+1)(L+2)} a_L$$

$$= -\frac{(l-L)(L+l+1)}{(L+1)(L+2)} a_L$$

As discussed earlier we have the even polynomials when $l = 2n$ i.e. $L = 2N = 0, 2, 4, \ldots 2n$ they obey the recursion relation with $n = 0, 1, 2, \ldots$

$$a_{2N+2} = -\frac{2(n-N)(2N+2n+1)}{(2N+2)(2N+1)} a_{2N}$$

So we have

N	
0	$a_2 = -2\,\frac{n(2n+1)}{2 \cdot 1} a_0$
1	$a_4 = -2\,\frac{(n-1)(2n+2+1)}{4 \cdot 3} a_2$
2	$a_6 = -2\,\frac{(n-2)(2n+4+1)}{6 \cdot 5} a_4$
3	$a_8 = -2\,\frac{(n-3)(2n+6+1)}{8 \cdot 7} a_6$
$\vdots$	

Thus we see that

$$a_{2N} = (-2)^N \frac{(n!)\,(2n+2N-1)!!}{(n-N)!\,(2N)!\,(2n-1)!!} a_0$$

Now note that

$$(2n+2N)! = (2n+2N)(2n+2N-1)(2n+2N-2)(2n+2N-3)\cdots$$

$$= (2n+2N)(2n+2N-2)\cdots\cdots 2 \quad \times$$
$$\times\ (2n+2N-1)(2n+2N-3)\cdots 1$$

$$= 2(n+N)2(n+N-1)\cdots 2(1)\times(2n+2N-1)!!$$

So $\quad (2n+2N-1)!! = \dfrac{(2n+2N)!}{2^{(n+N)}\,(n+N)!}$

and similarly

$$(2n-1)!! = \frac{(2n)!}{2^n\ n!}$$

Hence we secure

$$a_{2N} = (-2)^N \frac{n!}{(n-N)!\,(2N)!}\ \frac{(2n+2N)!\,2^n\,n!}{(n+N)!\,(2n)!\,2^{(n+N)}}\,a_0$$

$$= (-1)^N \frac{(2n+2N)!}{(2N)!\,(n+N)!\,(n-N)!}\left(\frac{n!\,n!}{(2n)!}\ a_0\right)$$

Since a_0 is arbitrary we absorb the $\dfrac{n!\,n!}{(2n)!}$ into it, $\dfrac{n!\,n!}{(2n)!}a_0 \longrightarrow a_0$

To obtain for $l = 2n$; $N = 1, 2, \ldots, n$

$$\boxed{a_{2N} = (-1)^N \frac{(2n+2N)!}{(2N)!\,(n+N)!\,(n-N)!}\, a_0}$$

For the odd polynomials $l = 2n+1$, $n = 0, 1, 2, \ldots$
and $L = 2N+1 = 1, 3, 5, \ldots$ i.e. $N = 0, 1, 2, \ldots$
we have

$$a_{2N+3} = -\frac{2(n-N)(2n+2N+3)}{(2N+3)(2N+2)}\, a_{2N+1}$$

So $\underline{N}$

0 $$a_3 = -2\,\frac{n(2n+3)}{3.2}\, a_1$$

1 $$a_5 = -2\,\frac{(n-1)(2n+2+3)}{5.4}\, a_3$$

2 $$a_7 = -2\,\frac{(n-2)(2n+4+3)}{7.6}\, a_5$$

⋮

We have then for $N = 0, 1, 2, \ldots, n$

$$a_{2N+1} = (-2)^N \frac{n!}{(n-N)!\,(2N+1)!} \, \frac{(2n+2N+1)!!}{(2n+1)!!} \, a_1$$

as before

$$(2m+2)! = 2^{m+1} (m+1)!\,(2m+1)!! \, .$$

Hence we secure

$$a_{2N+1} = (-1)^N \frac{(2n+2N+2)!}{(n+N+1)!\,(n-N)!\,(2N+1)!} \left(\frac{(n+1)!\,n!}{(2n+2)!} a_1 \right)$$

letting $\dfrac{(n+1)!\,n!}{(2n+2)!} a_1 \longrightarrow a_1$

we find for $l = 2n+1$, $n = 0, 1, 2, \ldots$ and $N = 1, 2, \ldots, n$

$$a_{2N+1} = (-1)^N \frac{(2n+2N+2)!}{(n+N+1)!\,(n-N)!\,(2N+1)!} \, a_1$$

We obtain the Legendre polynomial solutions for $P(\xi)$

For $l = 2n$, $n = 0, 1, 2, \ldots$

$$P_l(\xi) = a_0 \sum_{\substack{N=0 \\ (l=2n)}}^{n} (-1)^N \frac{(2n+2N)!}{(2N)!\,(n+N)!\,(n-N)!} \xi^{2N}$$

For $l = 2n+1$, $n = 0, 1, 2, \ldots$

$$P_l(\xi) = a_1 \sum_{\substack{N=0 \\ (l=2n+1)}}^{n} (-1)^N \frac{(2n+2N+2)!}{(2N+1)!\,(n+N+1)!\,(n-N)!} \xi^{2N+1} .$$

By convention $\boxed{a_0 \equiv \frac{(-1)^n}{2^{2n}} , \quad a_1 \equiv \frac{(-1)^n}{2^{2n+1}}}$

Hence the first few polynomials are

$P_0(\xi) = 1$

$P_1(\xi) = \xi$

$P_2(\xi) = \frac{1}{2}(3\xi^2 - 1)$

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

$\vdots$

Recall the properties of the Legendre polynomials:

1) $P_\ell(\xi)$ is Real

2) $P_\ell(-\xi) = (-1)^\ell P_\ell(\xi)$

3) $P_\ell(\xi)$ is a polynomial in ξ of degree ℓ.

4) $P_\ell(\pm 1) = (\pm 1)^\ell$

5) Rodrigues Formula:

$$P_\ell(\xi) = \frac{1}{2^\ell \ell!} \frac{d^\ell}{d\xi^\ell} (\xi^2 - 1)^\ell$$

Proof:
$$(\xi^2 - 1)^\ell = \sum_{m=0}^{\ell} \frac{(-1)^{\ell+m} \ell!}{m!(\ell-m)!} (\xi^2)^m$$

So
$$\frac{d^\ell}{d\xi^\ell} (\xi^2 - 1)^\ell = \sum_{\substack{m=n \\ \ell = \begin{cases} 2n \\ 2n-1 \end{cases}}}^{\ell} \frac{(-1)^{\ell+m} \ell!}{m!(\ell-m)!} (\xi)^{2m-\ell} \, 2m(2m-1) \cdots (2m-\ell+1)$$

Hence
$$\frac{d^\ell}{d\xi^\ell} (\xi^2 - 1)^\ell = \sum_{m=n}^{\ell} \frac{(-1)^{\ell+m} \ell!}{m!(\ell-m)!} \frac{(2m)!}{(2m-\ell)!} \xi^{2m-\ell}$$

Now analyzing the even and odd l case separately, we have

1) $l = 2n$; $2m - l = 2(m-n) \equiv 2N$, i.e. $N = m-n$, $N = 0, 1, \ldots, n$

So $l - m = n - N$, $m = N + n$ and we have

$$\frac{d^l}{d\xi^l}(\xi^2-1)^l = \sum_{N=0}^{n} \frac{(-1)^{N+n}\, l!\, (2N+2n)!}{(N+n)!\,(n-N)!\,(2N)!}\, \xi^{2N}$$

$$= l!\, 2^l P_l(\xi)$$

2) $l = 2n-1$; $2m - l = 2(m-n)+1 \equiv 2N+1 \Rightarrow N = m-n$

So $l - m = n - N - 1$, $m = n + N$ and we have

$$\frac{d^l}{d\xi^l}(\xi^2-1)^l = \sum_{N=0}^{n-1} \frac{(-1)^{N+n+1}\, l!\, (2N+2n)!}{(n+N)!\,(n-N-1)!\,(2N+1)!}\, \xi^{2N+1}$$

Letting $j = n-1$ (i.e. $n \to n+1$) and re-labelling j as n we have

$$\frac{d^l}{d\xi^l}(\xi^2-1)^l = l!\, 2^l P_l(\xi)$$, hence

the Rodrigues formula is verified.

6) Orthogonality

$$\int_{-1}^{+1} d\xi\, P_\ell(\xi) P_{\ell'}(\xi) = \frac{2}{2\ell+1}\delta_{\ell\ell'}$$

Proof: $(\ell \geq \ell')$

$$\int_{-1}^{+1} d\xi \frac{1}{2^\ell \ell!}\left[\frac{d^\ell}{d\xi^\ell}(\xi^2-1)^\ell\right] P_{\ell'}(\xi)$$

$$= \int_{-1}^{+1} d\xi \frac{(-1)^\ell}{2^\ell \ell!}(\xi^2-1)^\ell \frac{d^\ell}{d\xi^\ell} P_{\ell'}(\xi)$$

by integration by parts where the contribution from the endpoints vanishes since $P_{\ell'}(\pm 1) = (\pm 1)^{\ell'}$ and

$$\left.\frac{d^{\ell-n}}{d\xi^{\ell-n}}(\xi^2-1)^\ell\right|_{\xi=\pm 1} = 0, \quad 1 \leq n \leq \ell.$$ Now

$P_{\ell'}(\xi)$ is a polynomial in ξ of order ℓ'; hence this vanishes unless $\ell = \ell'$; From the series we have

$$P_\ell(\xi) = \frac{(2\ell)!}{2^\ell (\ell!)^2}\xi^\ell + O(\xi^{\ell-2})$$

Thus

$$\int_{-1}^{+1} d\xi\, P_\ell(\xi) P_{\ell'}(\xi) = \delta_{\ell\ell'} \frac{(-1)^\ell}{2^\ell \ell!} \ell! \frac{(2\ell)!}{2^\ell (\ell!)^2} \int_{-1}^{+1} d\xi (\xi^2-1)^\ell$$

$$= \delta_{\ell\ell'} \frac{(-1)^\ell (2\ell)!}{2^{2\ell} (\ell!)^2} \int_{-1}^{+1} d\xi (\xi^2-1)^\ell$$

and $\displaystyle\int_{-1}^{+1} d\xi (\xi^2-1)^\ell = \int_{-\pi/2}^{+\pi/2} d\theta\, (-1)^\ell \cos^{2\ell+1}\theta \qquad (\xi = \sin\theta)$

$$= (-1)^\ell\, 2 \int_0^{\frac{\pi}{2}} d\theta \cos^{2\ell+1}\theta = (-1)^\ell\, 2 \frac{(2\ell)!!}{(2\ell+1)!!}$$

$$= (-1)^\ell \frac{2^{\ell+1} \ell!}{(2\ell+1)!!} \qquad \text{since } (2\ell)!! = 2^\ell \ell!$$

So

$$\int_{-1}^{+1} d\xi\, P_\ell(\xi) P_{\ell'}(\xi) = \delta_{\ell\ell'} \frac{(2\ell)!\, 2^{\ell+1} \ell!}{2^{2\ell} (\ell!)^2 (2\ell+1)!!}$$

$$= \delta_{\ell\ell'} \frac{2}{2\ell+1} \underbrace{\frac{(2\ell)!}{2^\ell \ell! (2\ell-1)!!}}_{=1 \text{ (page -192-)}}$$

$$= \frac{2}{2\ell+1} \delta_{\ell\ell'}$$

as required.

7) Generating Function

$$Z(s) = \sum_{l=0}^{\infty} s^l P_l(\xi) = \frac{1}{\sqrt{1-2\xi s+s^2}}$$

So that

$$l!\, P_l(\xi) = \frac{\partial^l}{\partial s^l} Z(s)\Big|_{s=0} .$$

In addition to the Legendre functions, we define the associated Legendre functions $P_l^m(\xi)$ for $l=0,1,2,\ldots$ and $m=-l,-l+1,\ldots,0,+1,+2,\ldots,+l$.

$$\boxed{P_l^m(\xi) \equiv (1-\xi^2)^{\frac{|m|}{2}} \frac{d^{|m|}}{d\xi^{|m|}} P_l(\xi)}$$

Hence the polar angle eigenfunctions $\Theta(\xi)$ are given by the associated Legendre functions

$$\Theta_{lm}(\xi) = P_l^m(\xi) .$$

The properties of $P_l^m(\xi)$ follow from those of $P_l(\xi)$

1) $P_\ell^m(\xi)$ is real

2) $P_\ell^m(-\xi) = (-1)^{\ell+|m|} P_\ell^m(\xi)$.

3) $P_\ell^m(\xi) = P_\ell^{-m}(\xi)$

4) $P_\ell^0(\xi) = P_\ell(\xi)$

5) (Rodrigues) Formula

$$P_\ell^m(\xi) = \frac{(-1)^{|m|}(\ell+|m|)!}{2^\ell \ell!\,(\ell-|m|)!}(1-\xi^2)^{-\frac{|m|}{2}} \frac{d^{\ell-|m|}}{d\xi^{\ell-|m|}}(\xi^2-1)^\ell$$

6) Generating Function: differentiate the generating function for $P_\ell(\xi)$ $|m|$ times wrt ξ and multiply by $(1-\xi^2)^{\frac{|m|}{2}}$ yields

$$\sum_{\ell=|m|}^{\infty} P_\ell^m(\xi)\, s^\ell = \frac{(2|m|)!\,(1-\xi^2)^{\frac{|m|}{2}}\, s^{|m|}}{2^{|m|}(|m|)!\,(1-2\xi s+s^2)^{|m|+\frac{1}{2}}}$$

7) Orthogonality:

$$\int_{-1}^{+1} d\xi\, P_\ell^m(\xi)\, P_{\ell'}^m(\xi) = \frac{2}{2\ell+1}\frac{(\ell+|m|)!}{(\ell-|m|)!}\,\delta_{\ell\ell'}$$

8) Low order associated Legendre function

$$P_\ell^0(\xi) = P_\ell(\xi)$$

$$P_1^1(\xi) = \sqrt{1-\xi^2}$$

$$P_2^1(\xi) = 3\xi\sqrt{1-\xi^2}$$

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

$$\vdots$$

Hence, the angular eigenfunctions are given by $Y(\theta,\varphi) = \Theta(\cos\theta)\,\Phi(\varphi)$ and are labelled by the (ℓ, m) integers

$$\boxed{Y_\ell^m(\theta,\varphi) = A_{\ell m} P_\ell^m(\cos\theta)\, e^{im\varphi} \quad \text{with } \ell = 0,1,2,\ldots\ ;\ m = -\ell, -\ell+1, \ldots, 0, \ldots, \ell-1, \ell}$$

Where recall from page -181- the angular eigenvalue equations

1)
$$-i\frac{\partial}{\partial\varphi}Y_\ell^m(\theta,\varphi) = m\,Y_\ell^m(\theta,\varphi)$$
$$\Rightarrow\left(\frac{\partial^2}{\partial\varphi^2}+m^2\right)Y_\ell^m(\theta,\varphi)=0$$

2)
$$\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)-\frac{m^2}{\sin^2\theta}\right]Y_\ell^m(\theta,\varphi)$$
$$=-\ell(\ell+1)\,Y_\ell^m(\theta,\varphi)$$

Choosing the normalization constant $A_{\ell m}$ as

$$A_{\ell m}\equiv(-1)^{\frac{|m|+m}{2}}\left[\frac{2\ell+1}{4\pi}\,\frac{(\ell-|m|)!}{(\ell+|m|)!}\right]^{1/2},$$

the $Y_\ell^m(\theta,\varphi)$ are called the spherical harmonics. Their properties are given by those of P_ℓ^m and $e^{im\varphi}$:

1) Orthonormality

$$\int_{4\pi} d\Omega \, Y_\ell^{m*}(\theta,\varphi) Y_{\ell'}^{m'}(\theta,\varphi) = \delta_{\ell\ell'}\delta_{mm'}$$

where the solid angle integration is given by

$$\int_{4\pi} d\Omega \equiv \int_0^{2\pi} d\varphi \int_0^{\pi} d\theta \sin\theta$$

2) Low order spherical harmonics

$$Y_0^0(\theta,\varphi) = \frac{1}{\sqrt{4\pi}}$$

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

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

$$Y_2^{\pm 2}(\theta,\varphi) = \sqrt{\frac{15}{32\pi}} \sin^2\theta \, e^{\pm 2i\varphi}$$

$$Y_2^{\pm 1}(\theta,\varphi) = \mp\sqrt{\frac{15}{8\pi}} \sin\theta\cos\theta \, e^{\pm i\varphi}$$

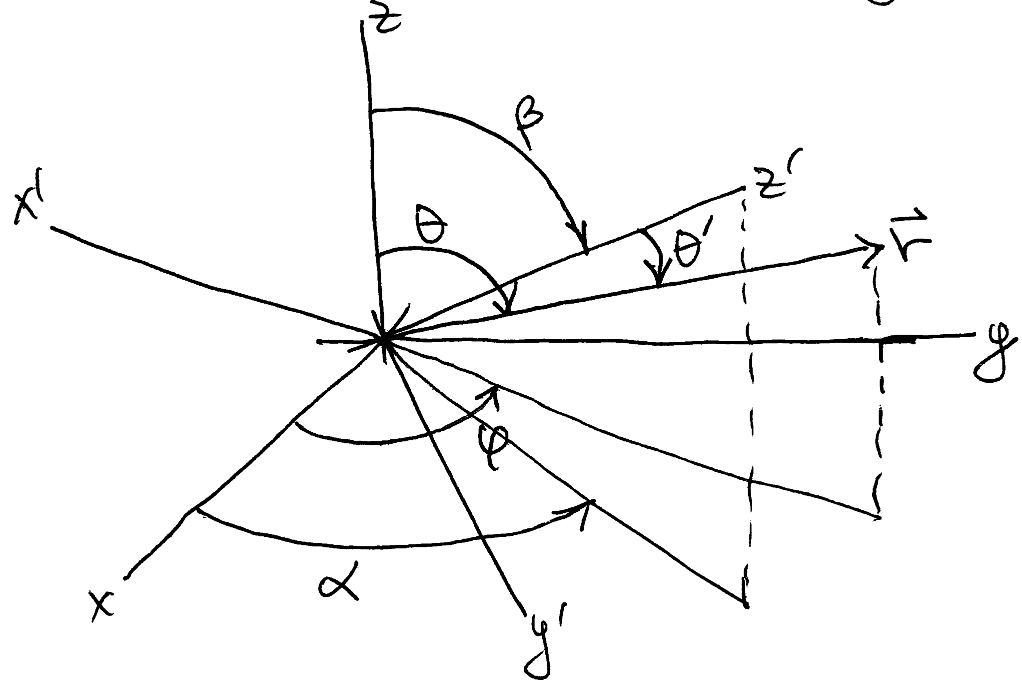
$$Y_2^0(\theta,\varphi) = \sqrt{\frac{5}{16\pi}} (3\cos^2\theta - 1)$$

$\vdots$

3) Addition Theorem For Spherical Harmonics

$$P_\ell(\cos\theta') = \frac{4\pi}{2\ell+1}\sum_{m=-\ell}^{+\ell} Y_\ell^{m*}(\beta,\alpha)\, Y_\ell^m(\theta,\varphi)$$

with the angles $\alpha, \beta, \theta, \varphi, \theta'$ given by



Finally, we have the energy eigenfunctions for a particle of mass m moving in a central potential $V = V(r)$ is

$$\psi_{\ell m} = R(r)\, Y_\ell^m(\theta,\varphi)$$

where $R(r)$ obeys the radial equation

$$\left(\frac{-\hbar^2}{2m}\right)\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}R(r)\right)+\left[V(r)+\frac{\hbar^2 \ell(\ell+1)}{2mr^2}\right]R(r)$$

$$= E R(r).$$

3.3. Orbital Angular Momentum

In classical mechanics the Hamiltonian for the central potential problem can be written as

$$H = \frac{p_r^2}{2m} + \frac{\vec{L}^2}{2mr^2} + V(r)$$

with p_r the momentum conjugate to r, $p_r = \frac{\partial \mathcal{L}}{\partial \dot{r}} = m\dot{r}$, while $\vec{L} = \vec{r} \times \vec{p}$ is the orbital angular momentum. Comparing this to the quantum mechanical Hamiltonian

$$H = -\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + V(r)$$

$$-\frac{\hbar^2}{2mr^2}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right]$$