When solving Schrödinger Equation for Hydrogen

$$\frac{\hbar^2 \nabla^2 \psi}{2m} + \frac{e^2}{r}\psi = E\psi \qquad \text{or}$$

$$\nabla^2 \psi + \frac{1}{\rho}\psi = \varepsilon \psi \qquad \text{in dimensionless form}$$

assume variables separable

$$\psi(\rho, \theta, \varphi) = R[\rho] \underbrace{\Theta(\theta)\, \Phi(\varphi)}_{Y(\theta,\varphi)}$$

where $\quad Y(\theta, \varphi) = y_{\ell m}(\theta) \times \begin{cases} \cos m\varphi \\ \sin m\varphi \end{cases}$

where $x = \cos\theta$ and $y_{\ell m}(\theta)$ can obey

$$\boxed{(1-x^2)\, y'' - 2xy' + \left[\ell(\ell+1) - \frac{m^2}{1-x^2}\right] y = 0} \quad m^2 \le \ell^2$$

This is Legendre's Associated Diff'y Eq

which agrees with ordinary Legendre iff $m = 0$

Hence

$$\boxed{y_{\ell, m=0} = P_\ell(x)}$$

magnetic quantum #

are special case solutions. $\quad -\ell \le m \le \ell$

To solve make the following substitution

$$\boxed{y = (1-x^2)^{m/2} u \equiv v^{m/2} u}$$

note $(v^{m/2})' = \frac{d}{dx}(1-x^2)^{m/2} = \frac{m}{2}(1-x^2)^{\frac{m}{2}-1}(-2x)$

$$= -xm(1-x^2)^{\frac{m}{2}-1}$$

$$= \boxed{-mx\, v^{\frac{m}{2}-1}}$$

and

$$(v^{m/2})'' = -m v^{\frac{m}{2}-1} - mx[v^{\frac{m}{2}-1}]'$$

$$= -m v^{\frac{m}{2}-1} - m(\tfrac{m}{2}-1)x\, v^{\frac{m}{2}-2}(-2x)$$

$$= \boxed{-m v^{\frac{m}{2}-1} + m(m-2)x^2 v^{\frac{m}{2}-2}}$$

Hence

$$y' = [u v^{m/2}]' = u'[v^{m/2}] + u[v^{m/2}]'$$

$$= \boxed{u' v^{m/2} + u[-mx\, v^{\frac{m}{2}-1}]}$$

$$y'' = [u\, v^{m/2}]''$$

$$= [u'' v^{m/2} + 2[u'][v^{m/2}]' + u[v^{m/2}]'']$$

$$= u'' v^{m/2} + 2u'[-mx\, v^{\frac{m}{2}-1}] + u[-m v^{\frac{m}{2}-1} + m(m-2)x v^{\frac{m}{2}-2}]$$

$$\Rightarrow v[u'' v^{m/2} + 2u'(-mx v^{\frac{m}{2}-1}) + u(-m v^{\frac{m}{2}-1} + m(m-2)x^2 v^{\frac{m}{2}-2})]$$

$$-2x[u' v^{\frac{m}{2}} + u[-mx\, v^{\frac{m}{2}-1})]]$$

$$+(\lambda - m^2 v^{-1})[v^{m/2} u] = 0$$

$$\Rightarrow [u'' v^{\frac{m}{2}+1} - 2mx u' v^{\frac{m}{2}} + (-m v^{\frac{m}{2}} + m(m-2)x^2 v^{\frac{m}{2}-1})u]$$

$$+[-2x u' v^{\frac{m}{2}} + (+2mx^2 v^{\frac{m}{2}-1})u]$$

$$+[+(\lambda v^{m/2} - m^2 v^{\frac{m}{2}-1})u] = 0$$

$$\Rightarrow \quad v^{\frac{m}{2}+1} u'' - 2(m+1) x u' v^{\frac{m}{2}} +$$

$$\left[(\lambda - m) v^{m/2} + (m(m-2)x^2 + 2m x^2 - m^2) v^{\frac{m}{2}-1} \right] u = 0$$

$$\Rightarrow \quad v\, v^{\frac{m}{2}} u'' - 2(m+1) x\, v^{\frac{m}{2}} u'$$

$$+ \left[(\lambda - m) v^{m/2} + (m^2 x^2 - \cancel{2m x^2} + \cancel{2m x^2} - m^2) v^{\frac{m}{2}-1} \right] u = 0$$

$$\Rightarrow \quad v\, v^{\frac{m}{2}} u'' - 2(m+1) x\, v^{\frac{m}{2}} u'$$

$$+ \left[(\lambda - m) v^{m/2} \qquad - m^2 \underbrace{(1-x^2)}_{v} v^{\frac{m}{2}-1} \right] u = 0$$

Divide by $v^{m/2}$

$$\Rightarrow \boxed{v u'' - 2(m+1) x u' + [\lambda - m(m+1)] u = 0} \qquad \text{Eq. } 10.3$$

If $m=0$ This reduces to

$$\boxed{(1-x^2) u_0'' - 2x u_0' + \lambda u_0 = 0}$$

Hence $\boxed{u_{\substack{\ell \\ m=0}} = P_\ell(x)}$

Differentiate Eq 10.3

$$v' u'' + v u''' - 2(m+1)[u' + x u''] + [\lambda - \overbrace{m(m+1)}^{\mu}] u' = 0$$

$$\Rightarrow \quad -2x u'' + v u''' - 2(m+1)[u' + x u''] + [\lambda - \mu] u' = 0$$

$$\Rightarrow \quad v u''' + [-2(m+1)x - 2x] u'' + [\lambda - \mu - 2(m+1)] u' = 0$$

$$\Rightarrow \quad (1-x^2)(u')'' - 2[(m+1)+1] x (u')' + [\lambda - (m(m+1) + 2(m+1))](u') = 0$$

$$\Rightarrow \boxed{(1-x^2)[u']'' - 2[(m+1)+1] x [u']' + [\lambda - (m+1)(m+2)] [u]' = 0}$$

Eq. 10.4

which means u' is a solution to Eq 10.3 with $m \to m+1$ That is

$u = P_\ell(x)$ is a solution with $m=0$

$u' = P_\ell'(x)$ is a solution with $m=1$

$\vdots$

$u^{(m)} = P_\ell^{(m)}(x)$ is a solution with $m=m$

That is $u_m = \frac{d^m}{dx^m} P_\ell(x) \quad \forall \ell, m$ Eq 10.3

and
$$\boxed{y = (1-x^2)^{m/2} \frac{d^m}{dx^m} P_\ell(x) \equiv P_\ell^m}$$ Eq. 10.1

This is a Rodriques Formula for associated Legendre. Typically $\ell = 0, 1, 2, \ldots$

$-\ell \le m \le \ell$

Also Recall

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

$$\Rightarrow \quad \boxed{P_\ell^m(x) \equiv \frac{1}{2^\ell \ell!} (1-x^2)^{\frac{m}{2}} \frac{d^{\ell+m}}{dx^{\ell+m}} (x^2-1)}$$

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

$P_0^0 = 1$; $P_1^0 = x$; $P_1^1 = (1-x^2)^{1/2}$ etc.

The associated Legendre are reparameterized in terms of $x = \cos\theta$

which gives $1 - x^2 = 1 - \cos^2\theta = \sin\theta$

and the Rodriques Formula Becomes

$$\boxed{P_\ell^m(\theta) = [\sin\theta]^m \frac{d^m}{d[\cos\theta]^m} P_\ell[\cos\theta]}$$

$P_0^0(\theta) = 1$

$P_1^0(\theta) = \cos\theta$

$P_1^1(\theta) = \sin\theta$

$P_2^0(\theta) = \frac{3}{2}\cos^2\theta - \frac{1}{2}$

$P_2^1(\theta) = 3\cos\theta\sin\theta$

$P_2^2(\theta) = 3\sin^2\theta$

$dx = -\sin\theta\, d\theta$
$x = \cos\theta$
$x: -1 \to 1$
$\theta: \pi \to 0$

The angular orthonormality condition gives

$$\boxed{\int_0^\pi P_\ell^m(\theta)\, P_{\ell'}^m(\theta) \sin\theta\, d\theta = \frac{2}{2\ell+1} \frac{(\ell+m)!}{(\ell-m)!} \delta_{\ell\ell'}}$$

These are used to solve the wave Eq. in spherical coordinates:

$$\boxed{\nabla^2 \Psi(\theta, \varphi) + \lambda \Psi = 0}$$ where $\lambda = \ell(\ell+1)$

whith $\nabla^2 \psi = \frac{\partial^2 \psi}{\partial \theta^2} + \cot\theta \frac{\partial \psi}{\partial \theta} + \csc^2\theta \frac{\partial^2 \psi}{\partial \varphi^2}$

setting $r=1$ on surface of unit sphere

Hence Wave Eq. $\nabla^2 \psi + \lambda \psi = 0$

$$\Rightarrow \frac{\partial^2 \psi}{\partial \theta^2} + \cot\theta \frac{\partial \psi}{\partial \theta} + \csc^2\theta \frac{\partial^2 \psi}{\partial \varphi^2} + \lambda \psi = 0$$

$$\psi = \Theta(\theta)\, \Phi(\varphi)$$

$$\Rightarrow \Theta'' + \cot\theta\, \Theta' + \left[\lambda - \frac{m^2}{\sin^2\theta} \right] \Theta = 0 \qquad A.L.P.Q$$

$$\Phi'' + m^2 \Phi = 0 \qquad \text{where } -l \le m \le l$$

$$\Rightarrow \Theta = P_l^m(\cos\theta)$$

$$\Phi = e^{im\varphi}$$

$$\Rightarrow \psi_l^m = N\, P_l^m[\cos\theta] * e^{im\varphi}$$

$$N^2 \Rightarrow 1 = \int \psi^* \psi \, d\Omega = \int_{SA} \psi^* \psi \sin\theta \, d\theta \, d\varphi$$

$$= N^2 \int P_l^m P_l^m \sin\theta \, d\theta \, d\varphi \qquad \int_0^{2\pi} d\varphi = 2\pi$$

$$= N^2 \cdot 2\pi \cdot \frac{2}{2l+1} \frac{(l+m)!}{(l-m)!}$$

$$\Rightarrow N_l^m = \sqrt{\frac{2l+1}{4\pi} \frac{(l-m)!}{(l+m)!}} \Rightarrow \boxed{Y_l^m \equiv N_l^m P_l^m[\cos\theta]\, e^{im\varphi}}$$

$$\equiv \psi_l^m$$