hydrogen atom R_{20} and R_{21} derivation

Recap wave function

$$\Psi(n l m) = R(r)_{nl} \times Y_l^m(\theta, \phi)$$

$$R_{nl} = \frac{u}{r}$$

$$= \frac{(e^{-\delta})(\delta^{l+1})\, v(\delta)}{r}$$

$$v(\delta) = \sum_{j=0}^{\infty} C_j \delta^j$$

$\boxed{C_0}$

$$C_{j+1} = \left[\frac{2(j+l+1)-n}{(j+1)(j+2l+2)} C_j\right]$$

$\therefore J_{max} = n - l$

$\Psi_{100} :- (r, \theta, \phi) = R_{10} Y_0^0 \to \frac{1}{\sqrt{4\pi}}$

$\Psi_{100} :- \frac{1}{\sqrt{\pi a^3}} e^{-r/a}$

$\cancel{\Psi_{110}}$ and $\cancel{\Psi_{111}}$ $\quad l < n$

$l = n$

$\boxed{l = 1 \quad n = 1}$

$f(l) = n$

$1 = 1 - 1 - J_{max}$

$[J_{max} = \text{negative}]$ ✗

—x——x———x———x———x———x———x—

$\boxed{R_{20}, R_{21}}$: not normalizing method

↳ complicated

R_{20} : $n = 2, l = 0$ $\quad$ $J_{max} = n - l - 1$

$= 2 - 0 - 1$

$J_{max} = 1$

$J_{max} = \sum_0^1$

$\therefore \sum_0^1 C_j S^j$

$= C_0 (S^0) + C_1 (S^1)$

$= C_0 + C_1 S$

$\boxed{C_1 = -C_0}$

$$C_{j+1} = \frac{2(j + l + 1 - n)}{(j+1)(j+2l+2)} C_j$$

$$C_1 = \frac{2[0 + 0 + 1 - 2]}{[1+1][1+2(0)+2]} C_0$$

$$C_1 = \frac{2[-1]}{[2][3]}$$

$$C_1 = \frac{-1}{3} C_0$$

$$\boxed{C_1 = -\frac{1}{3} C_0}$$

$R_{n l}$ $l=0$

$C_1 = -C_0$

$\therefore v(\delta) = C_0 - C_0\delta$

$= C_0(1-\delta)$

R/C $\therefore R_{nl} = \left[\frac{1}{r} e^{-\delta} \delta^{(l+1)} v(\delta)\right]$

$R_{nl} = \left[\frac{1}{r} e^{-\delta} \delta^{(l+1)}\right]\left[C_0(1-\delta)\right]$

$\delta = \frac{r}{a_n} \quad \frac{r}{2a}$

$R_{n1} = \left[\frac{1}{r}\delta e^{-\delta}\right]\left[C_0(1-\delta)\right]$

$R_{n1} = \left[\frac{1}{r}\frac{r}{2a} e^{-\delta}\right]\left[C_0(1-\delta)\right]$

$R_{n1} = \left[\frac{\cancel{r}\,1}{2a\cancel{r}} e^{-\delta}\right]\left[C_0(1-\delta)\right]$

$R_{20} = \frac{C}{2a}\left(1-\frac{r}{2a}\right) e^{-r/2a}$

—x—x—x—x—x—x—x—

Derivation of R_{21}

$n = 2 \quad l = 1$

$J_{max} = n - l - 1$

$= 2 - 1 - 1$

$J_m \qquad J_{max} = 0$

$$v(\delta) = C_0$$

$$\sum_{0}^{0} C_j \delta^j \quad C_0 \delta^0 = C_0(1) = C_0$$

$$= \frac{1}{r} \cdot \delta^2 e^{-\delta} C_0 = \frac{C_0}{\cancel{r}} \frac{r^{\cancel{2}}}{4a^2} e^{-r/2a}$$

$$\boxed{= \frac{C_0 r}{4a^2} e^{-r/2a}}$$

—X——X——X——X——X——

R_{20} and R_{21} derivation using maths

Legendre polynomials

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

$$P_1(x) = \frac{1}{2^{(1)} l!} \left(\frac{d}{dx}\right)^1 (x^2-1)^1$$

$P_0(x) = 1$

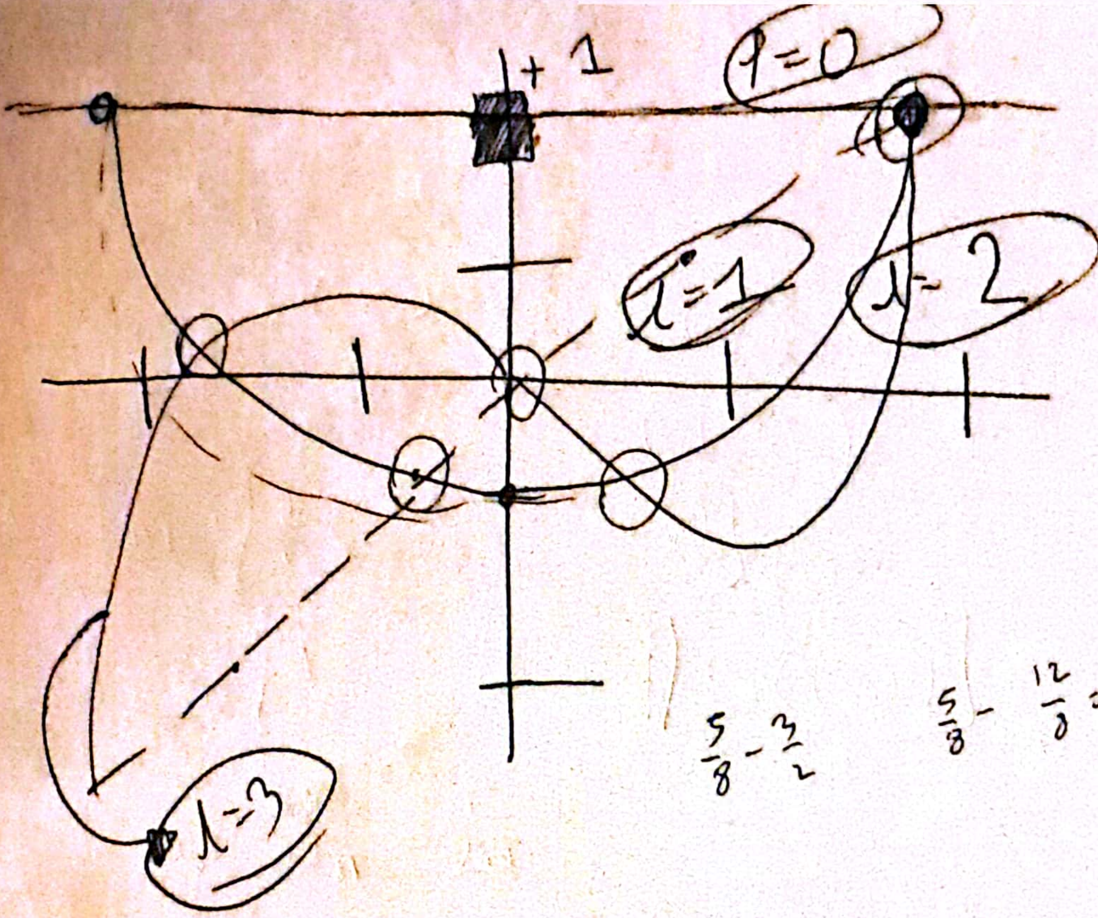
$P_1(x) = x$

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

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

$P_4(x) = \frac{1}{8}(35x^4-30x^2+3)$

[graph in next page]



$\frac{5}{8} - \frac{3}{2}$ $\qquad$ $\frac{5}{8} - \frac{12}{8} = -\frac{7}{8}$

$= -\frac{7}{16}$

$x = \frac{1}{2}$ $\quad \frac{1}{2}(3(\frac{1}{2})^2 - 1)$ $\qquad \frac{1}{2}(3-1)$

$\frac{1}{2}(\frac{3}{4}) - 1)$

$\frac{1}{2}(-\frac{1}{4})$ $\qquad P_3(x) = \frac{1}{2}(5x^3 - 3x)$

$-\frac{1}{8}$

$n = 1$ 1 node
$n = 2$ 2 node
$n = 3$ 3 nodes

Associated legendre polynomials

$$P_\ell^m(x) \equiv (1-x^2)^{\frac{|m|}{2}} \left(\frac{d}{dx}\right)^{|m|} P_\ell(x)$$

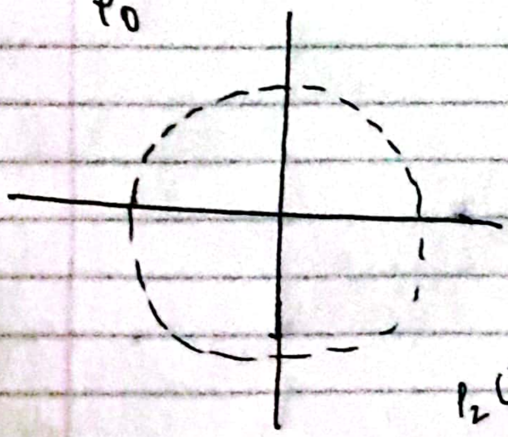
$\boxed{x = \cos(\theta)}$

- $P_0^0 = 1 = 1$
- $P_1^0 = x = \cos(\theta)$
- $P_1^1 \equiv \sqrt{1-x^2} = \sin(\theta)$
- $P_2^0 = \frac{1}{2}(3x^2-1)$

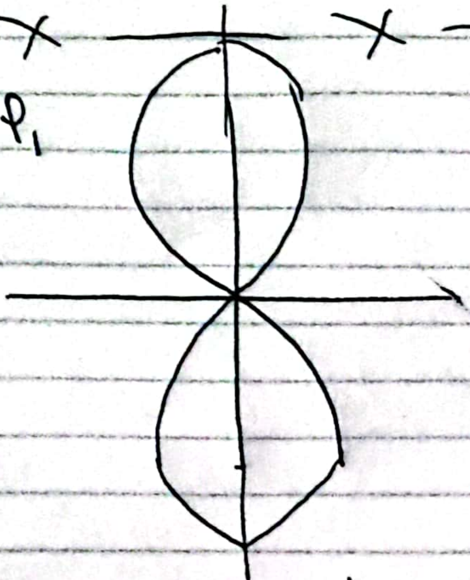
$P_2^1 = 3x\sqrt{1-x^2} = 3\sin(\theta)\cos(\theta)$

$P_2^2 = 3(1-x^2) = 3\sin^2\theta$

P_0



P_1



P_2^0

P_1^1