Appendix A: Solving the θ-equation for $m_\ell = 0$ case

- Using $v = \cos\theta$, $P(v) \equiv \Theta(\theta)$

θ-eq:
$$\frac{d}{dv}\left[(1-v^2)\frac{dP}{dv}\right] + \left(\lambda - \frac{m_\ell^2}{1-v^2}\right)P = 0 \quad (A1)$$

Each m_ℓ value gives an equation for $P(v)$

General m_ℓ, complicated

Here, we illustrate the path to solving $m_\ell = 0$ case.

Another reason: Solutions are useful in EM

Put $m_\ell = 0$,
$$\frac{d}{dv}\left[(1-v^2)\frac{dP}{dv}\right] + \lambda P = 0 \quad (A2)$$

[An eigenvalue problem, λ (or $-\lambda$) is eigenvalue]

Series Solution to (A2)

Step 1
$$P(v) = \sum_{p=0}^{\infty} a_p v^p \quad (A3) \quad [v = \cos\theta]$$

[Think: Look for recursive relation of coefficients]

$$\frac{dP}{dv} = \sum_{p=0}^{\infty} a_p\, p\, v^{p-1}$$

$$\frac{d}{dv}\left[(1-v^2)\frac{dP}{dv}\right] = \frac{d}{dv}\sum_{p=0}^{\infty}\left[a_p\, p\, v^{p-1} - a_p\, p\, v^{p+1}\right]$$

$$= \sum_{p=0}^{\infty} a_p\, p(p-1)\, v^{p-2} - \sum_{p=0}^{\infty} a_p\, p(p+1)\, v^p$$

$$= \sum_{p=2}^{\infty} a_p\, p(p-1)\, v^{p-2} - \sum_{p=0}^{\infty} a_p\, p(p+1)\, v^p$$

$$= \sum_{p=0}^{\infty}\left[a_{p+2}(p+2)(p+1) - a_p\, p(p+1)\right] v^p$$

$$\text{Eq. (A2)} \Rightarrow \sum_{p=0}^{\infty}\Big[\underbrace{a_{p+2}(p+2)(p+1) - a_p\big(p(p+1)-\lambda\big)}_{=\,0}\Big] v^p = 0$$

($\because$ v^p different p's are independent)

$$\boxed{\frac{a_{p+2}}{a_p} = \frac{p(p+1)-\lambda}{(p+1)(p+2)}} \qquad \text{(A4)}$$

Recursive relation

<u>Meaning</u>: (i) Know $a_0 \to a_2 \to a_4 \to \cdots$

Know $a_1 \to a_3 \to a_5 \to \cdots$

(ii) From experience in oscillator problem, numerator will impose $\lambda = p(p+1)$ $[p = 0, 1, 2, \cdots]$ for acceptable behavior

Step 2: $\frac{a_{p+2}}{a_p} \sim \frac{p^2}{p^2} \to 1$ $\underbrace{(p \to \infty \text{ limit})}_{\text{if (A3) is really an infinite series}}$

Step 3: Look for a function of similar behavior when expressed as an infinite series

Consider $\frac{1}{1-v} = \sum_{p=0}^{\infty} v^p$ $\underbrace{\text{(all coefficients are 1)}}_{\frac{a_{p+2}}{a_p} = 1}$

$\therefore$ Eq. (A3) behaves as $\frac{1}{1-v}$

This is bad because $\frac{1}{1-v}$ diverges at $\underset{\cos\vartheta}{v} = 1$

If so, $P(v)$ and so $\underbrace{\psi(\vec{r}) \text{ diverges!}}_{\text{not well-behaved}}$

Step 4: Infinite Series in Eq. (A3) is bad.

Way Out? See Eq. (A4), terminate infinite series and turn it into a polynomial.

- This happens only when λ (eigenvalue in Eq. (A2)) hits at values that numerator of Eq. (A4) vanishes.

$\therefore$ λ must be of the form

$$\boxed{\lambda = \ell(\ell+1)} \qquad \text{(A5)}$$

$\ell = 0, 1, 2, 3, \cdots$ (integers)

- E.g. If $\lambda = 12 = 3\times4$ $(\ell=3)$

  From Eq. (A4), $a_3 \neq 0$, but $a_5, a_7, a_9, \cdots = 0$

  $\therefore$ $P_3(v) = a_1 v + a_3 v^3$ (a polynomial)

  connected by Eq. (A4)

  (this P_3 is odd in v and highest term $\sim v^3$)

- E.g. If $\lambda = 20 = 4\times5$ $(\ell=4)$

  $a_4 \neq 0$, but $a_6, a_8, a_{10}, \cdots = 0$

  $\therefore$ $P_4(v) = a_0 + a_2 v^2 + a_4 v^4$

  Connected by Eq. (A4)

  (this P_4 is even in v and highest term $\sim v^4$)

From Eq.(A3), write

$$P(v) = a_0\underbrace{\left(1 + a_2' v^2 + a_4' v^4 + \cdots\right)}_{\text{even in } v} + a_1\underbrace{\left(v + a_3' v^3 + a_5' v^5 + \cdots\right)}_{\text{odd in } v}$$

- If ℓ is odd, odd part terminates into a polynomial (OK)
  Even part cannot terminate (bad), kill it by $a_0 = 0$
  Result: $P_{\ell=odd}(v)$ is an odd function (highest term v^ℓ)
- If ℓ is even, even part terminates into a polynomial (OK)
  Odd part cannot terminate (bad), kill it by $a_1 = 0$
  Result: $P_{\ell=even}(v)$ is an even function (highest term v^ℓ)
- The solution labelled by ℓ is:
  $P_\ell(v)$ [Legendre Polynomials] $(P_\ell(\cos\theta))$

A few $P_\ell(v)$: $$P_0(v) = 1$$
$$P_1(v) = v$$
$$P_2(v) = \frac{1}{2}(3v^2 - 1) \qquad (A6)$$
$$P_3(v) = \frac{1}{2}(5v^3 - 3v)$$
$$\vdots$$

By convention: $P_\ell(v) = a_\ell v^\ell + a_{\ell-2} v^{\ell-2} + \cdots$

taken to be $\frac{(2\ell)!}{2^\ell (\ell!)^2}$

Summary

$P_\ell(v)$ satisfies Eq. (A2), i.e.

$$\frac{d}{dv}\left[(1-v^2)\frac{dP_\ell}{dv}\right] + \ell(\ell+1)P_\ell = 0 \qquad (A7)$$

This is how $P_\ell(\cos\theta)$ comes about.

Associated Legendre Polynomials

Eq. (A1): $$\frac{d}{dv}\left[(1-v^2)\frac{dP}{dv}\right] + \left[\lambda - \frac{m_\ell^2}{1-v^2}\right]P = 0 \qquad (A1)$$

- m_ℓ^2 appears $\Rightarrow$ solutions labelled by ℓ and $|m_\ell|$

Solutions $P_\ell^{|m|}(v)$ given by

$$\boxed{P_\ell^{|m|}(v) = (1-v^2)^{\frac{|m_\ell|}{2}} \frac{d^{|m|}}{dv^{|m|}} P_\ell(v)} \qquad (A8)$$

known

<u>Ex:</u> Check (A8) is a solution by direct substitution into (A1)

Since $P_\ell(v) \sim v^\ell + \cdots$

If $|m_\ell| > \ell$, then $P_\ell^{|m|}(v) = 0$ ($\psi = 0$ bad)

$\therefore$ m_ℓ (for a given ℓ) satisfies the condition

$$\underbrace{-\ell \le m_\ell \le \ell}_{(2\ell+1) \text{ values of } m_\ell \text{ for a given } \ell} \qquad (m_\ell \text{ integers}) \qquad (A9)$$

Spherical Harmonics

$$Y(\theta,\phi) \sim P_\ell^{|m|}(\cos\theta)\cdot e^{im_\ell\phi}$$

Normalizing $Y(\theta,\phi)$ over ranges for θ and ϕ,

$$\boxed{\begin{aligned} Y_{\ell m}(\theta,\phi) &= (-1)^m\left[\frac{2\ell+1}{4\pi}\frac{(\ell-|m|)!}{(\ell+|m|)!}\right]^{1/2} P_\ell^{|m|}(\cos\theta)\, e^{im\phi} \quad (\text{for } m\geq 0) \\ \text{and } Y_{\ell\, -m}(\theta,\phi) &= (-1)^m\, Y_{\ell m}(\theta,\phi) \end{aligned}} \qquad (10)$$

This is the complete mathematical definition of <u>Spherical Harmonics</u>.

Key Take-Home Message

- As long as $U = U(r)$, then TISE's solutions

$$\psi(r,\theta,\phi) \sim R(r)\cdot \underbrace{Y_{\ell m_\ell}(\theta,\phi)}_{\substack{\text{always there regardless of the}\\ \text{explicit form of } U(r)\\ [\text{only needed spherically symmetric } U(r)]}}$$