

2012. 5. 16. QM 1. (Grad)

$$\mathcal{Q}_{\Theta} = \frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \left(\sin\theta \frac{\partial}{\partial\theta} \right) + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2}$$

$$\left(\mathcal{Q}_{\Theta} + l(l+1) \right) \Theta = 0.$$

$$\downarrow$$
$$\left[\underbrace{\sin\theta \frac{\partial}{\partial\theta} \left(\sin\theta \frac{\partial}{\partial\theta} \right) + l(l+1) \sin^2\theta}_{\Theta \text{ dependent}} + \underbrace{\frac{\partial^2}{\partial\phi^2}}_{\phi \text{ dependent}} \right] \Theta = 0.$$

$$\therefore \Theta = A(\theta) \Phi(\phi)$$

$$\Phi \left[\sin\theta \frac{\partial}{\partial\theta} \left(\sin\theta \frac{\partial A}{\partial\theta} \right) + l(l+1) \sin^2\theta A \right] + A \cdot \frac{\partial^2 \Phi}{\partial\phi^2} = 0$$

Dividing by $A\Phi$,

$$\therefore \frac{\sin\theta \frac{d}{d\theta} \left(\sin\theta \frac{dA}{d\theta} \right) + l(l+1) \sin^2\theta A}{A} = - \frac{\frac{d^2\Phi}{d\phi^2}}{\Phi} = \text{Const.}$$

(ind. of θ & ϕ)

ϕ dependence

$$\langle r, \theta, \phi | L_z | n, l, m \rangle$$

coordinate space representation
 $L_z = \frac{\hbar}{i} \frac{\partial}{\partial \phi}$

$$= \frac{\hbar}{i} \frac{\partial}{\partial \phi} \langle r, \theta, \phi | n, l, m \rangle$$

$$= m\hbar \langle r, \theta, \phi | n, l, m \rangle$$

$$= \langle r, \theta, \phi | m\hbar | n, l, m \rangle$$

Since.. $\langle r, \theta, \phi | n, l, m \rangle = R_{nl}(r) \Theta(\theta) \Phi(\phi)$

Φ dependence appears here only!

$$\therefore \frac{\hbar}{i} \frac{\partial}{\partial \phi} \Phi(\phi) = m\hbar \Phi(\phi)$$

$$\therefore \frac{d^2 \Phi}{d\phi^2} = -m^2 \Phi$$

$$-\frac{1}{\Phi} \frac{d^2 \Phi}{d\phi^2} = m^2$$

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$\theta$  dependence

~~$\sin \theta \frac{\partial}{\partial \theta}$~~

$$\sin \theta \frac{d}{d\theta} \left( \sin \theta \frac{dA}{d\theta} \right) + l(l+1) \sin^2 \theta A - m^2 A = 0$$

$$\therefore \frac{1}{\sin\theta} \cdot \frac{d}{d\theta} \left( \sin^2\theta \frac{1}{\sin\theta} \frac{dA}{d\theta} \right) + \left( l(l+1) - \frac{m^2}{\sin^2\theta} \right) A = 0.$$

$$\begin{cases} x = \cos\theta \\ dx = -\sin\theta d\theta \\ \sin^2\theta = 1-x^2 \end{cases}$$

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

⇓ (Associated Legendre equation)

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

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$$\frac{\hbar^2}{\lambda} \frac{d}{d\phi} \Phi(\phi) = m\hbar \Phi(\phi) \rightarrow \Phi \propto e^{im\phi}$$

$$\therefore \Psi = A(\theta) \Phi(\phi) \propto P_l^m(\cos\theta) e^{im\phi}$$

↓ normalization

$$Y_l^m(\theta, \phi) = \langle \hat{n}(\theta, \phi) | l, m \rangle \quad \begin{matrix} \rightarrow (r \text{ is decoupled}) \\ (V(\vec{r}) \Rightarrow V(r)) \end{matrix}$$

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$$Y_{lm}(\theta, \varphi)$$

The complete form?

$$l+m+1.$$

$$Y_{ll}(\theta, \varphi) = \langle \hat{n}(\theta, \varphi) | ll \rangle$$

↓

$$Y_{lm}(\theta, \varphi) = \boxed{\phantom{0}} \langle \hat{n}(\theta, \varphi) | L_-^{l-m} | ll \rangle$$

$$l - (l-m) = m.$$

$$\left\{ \begin{array}{l} |L_{-1}lm\rangle|^2 = \langle lm | L_+ L_- |lm\rangle \\ L_- |lm\rangle = \hbar \sqrt{(l+m)(l-m+1)} |l, m-1\rangle \end{array} \right\}$$

$$L_- |ll\rangle = \hbar \sqrt{(l+l)(l-l+1)} |ll-1\rangle = \hbar \sqrt{2l \cdot 1} |ll-1\rangle$$

$$\begin{aligned} (L_-)^2 |ll\rangle &= \hbar \sqrt{(l+l)(l-l+1)} \cdot \hbar \sqrt{(l+l-1)(l-l+1+1)} |ll-2\rangle \\ &= \hbar^2 \sqrt{2l \cdot 1} \cdot \sqrt{2l-1 \cdot 2} |ll-2\rangle \end{aligned}$$

$$\begin{aligned} \vdots \\ (L_-)^{l-m} |ll\rangle &= (\hbar)^{l-m} \cdot \sqrt{2l \cdot (2l-1) \cdot \dots \cdot (2l - (l-m+1))} \\ &\quad \cdot \sqrt{1 \cdot 2 \cdot \dots \cdot (l-m)} |lm\rangle \end{aligned}$$

$$= (\hbar)^{l-m} \sqrt{\frac{(2l)! (l-m)!}{(l+m)!}} |lm\rangle$$

$$\therefore |l, m\rangle = \left(\frac{L_-}{\hbar}\right)^{l-m} |l, l\rangle \cdot \sqrt{\frac{1}{(2l)!} \cdot \frac{(l+m)!}{(l-m)!}}$$

$$\underbrace{|l, l\rangle}_{??}$$

$$L_+ |l, l\rangle = 0 \quad (\text{d. } a_{10} = 0)$$

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

Explicitly..

$$\langle \tilde{x} | L_+ | \alpha \rangle = \hbar e^{i\phi} \left( \frac{\partial}{\partial \theta} + i \cot \theta \frac{\partial}{\partial \phi} \right) \langle \tilde{x} | \alpha \rangle \quad \rightarrow \langle r, \hat{n}(\theta, \phi) |$$

$$\therefore \hbar e^{i\phi} \left( \frac{\partial}{\partial \theta} + i \cot \theta \frac{\partial}{\partial \phi} \right) Y_{ll}(\theta, \phi) = 0$$

$$\frac{\hbar}{i} \frac{\partial}{\partial \phi} Y_{ll} = \hbar l Y_{ll}$$

$$\therefore \frac{\partial}{\partial \theta} + i \cot \theta \frac{\partial}{\partial \phi}$$

$$\left( \frac{\partial}{\partial \theta} + i \cot \theta \cdot \frac{i m \hbar}{\hbar} l \right) Y_{ll} = 0$$

$$\therefore \left( \frac{\partial}{\partial \theta} - l \cot \theta \right) Y_{ll} = 0$$

$$\underline{Y_{\ell m}(\theta, \phi) = f(\theta) e^{im\phi}}$$

$$\therefore \left( \frac{d}{d\theta} - \ell \cot \theta \right) f(\theta) = 0.$$

$$\therefore \frac{df}{d\theta} = \ell \frac{\cos \theta}{\sin \theta} f(\theta).$$

$$\underline{\cos \theta d\theta = d(\sin \theta)^x}$$

$$\frac{df(\theta)}{d(\sin \theta)} = \frac{\ell}{\sin \theta} f(\theta).$$

$$\therefore \frac{df}{dx} = \frac{\ell}{x} f. \quad \rightarrow \quad \frac{df}{f} = \ell \cdot \frac{dx}{x}$$

$$\log \frac{f}{f_0} = \ell \cdot \log \frac{x}{x_0}$$

$$\Rightarrow \frac{f}{f_0} = \frac{f_0 x^\ell}{f_0 x_0^\ell} \quad f(x) = N \cdot x^\ell$$

normalization  
↑  
-tion

$$\therefore \frac{f}{f_0}$$

$$\therefore f(\theta) = \underset{\substack{I \\ \theta}}{N} \cdot x^\ell = C_\ell x^\ell = C_\ell \cdot \sin^\ell \theta.$$

$$\therefore Y_{\ell\ell}(\theta, \varphi) = C_{\ell} \sin^{\ell} \theta e^{im\varphi}$$

$$\langle \alpha | \alpha \rangle = 1.$$

$$\langle \alpha | \int d^3x |\vec{x}\rangle \langle \vec{x} | \alpha \rangle = 1.$$

$$\left( |r, \hat{n}(\theta, \varphi)\rangle = |r\rangle \otimes |\hat{n}(\theta, \varphi)\rangle \right)$$

$V(\vec{r}) = V(r)$

$$\left[ \int_0^{\infty} dr r^2 |r\rangle \langle r| \int d\Omega |\hat{n}\rangle \langle \hat{n}| \right]$$

$(\int_{-1}^1 d\cos\theta \int_0^{2\pi} d\varphi = \int d\Omega = 4\pi)$

$$\langle \ell m | \ell m \rangle = 1$$

↓

$$\langle \ell m | \int d\Omega |\hat{n}\rangle \langle \hat{n} | \ell m \rangle = \int d\Omega \langle \ell m | \hat{n} \rangle \langle \hat{n} | \ell m \rangle = 1$$

$$\int d\Omega \langle \ell \ell | \hat{n} \rangle \langle \hat{n} | \ell \ell \rangle = 1.$$

$$\int d\Omega Y_{\ell\ell}^*(\theta, \varphi) Y_{\ell\ell}(\theta, \varphi) = 1$$

$$\int_{-1}^1 d\cos\theta \int_0^{2\pi} d\phi (4\pi)^{-1} \cdot \underbrace{(\sin^2\theta)^l}_{(1-x^2)} = 1. \quad x = \cos\theta.$$

$$= (4\pi)^{-1} \cdot 2\pi \cdot \int_{-1}^1 dx (1-x^2)^l = 1.$$

↓

$$4\pi (4\pi)^{-1} \int_0^1 dx (1-x^2)^l = 1.$$

$$x^2 = t \quad x = t^{1/2}$$

$$2x dx = dt$$

$$dx = \frac{dt}{2x} = \frac{1}{2} t^{-1/2} dt$$

~~$$\int_0^1 dx$$~~

$$\int_0^1 dx (1-x^2)^l = \int_0^1 dt \cdot \frac{t^{-1/2}}{2} \cdot (1-t)^l$$

$$= \frac{1}{2} \int_0^1 dt t^{\frac{1}{2}-1} (1-t)^{(l+1)-1}$$

$$= \frac{1}{2} \cdot B\left(\frac{1}{2}, l+1\right) = \frac{\Gamma\left(\frac{1}{2}\right) \Gamma\left(l+\frac{1}{2}\right)}{2 \cdot \Gamma\left(l+\frac{3}{2}\right)}$$

이런게도 풀 수 있다. 있다고  
 하지만 지금은 이렇게



$$2\pi |C_l|^2 \int_{-1}^1 dx (1-x^2)^l = 1.$$

$$\left( \begin{array}{l} dx = 2dt \\ 1+x = 2t \\ x = 2t-1 \\ 1-x = 2-2t \\ 1-x^2 = 4t(1-t) \end{array} \right)$$

$$\rightarrow 2\pi |C_l|^2 \int_0^1 (2dt) [4t(1-t)]^l$$

$$= \cancel{2}^{2l+1}$$

$$= 2\pi |C_l|^2 \cdot 2^{2l+1} \cdot B(l+1, l+1)$$

$$= 2\pi |C_l|^2 \cdot 2^{2l+1} \cdot \frac{\Gamma(l+1)\Gamma(l+1)}{\Gamma(2l+2)}$$

$$= 1.$$

$$\therefore |C_l|^2 = \frac{(2l+1)!}{4\pi \cdot 2^{2l} \cdot (l!)^2}$$

$$Y_{ll}(\theta, \phi) = \sqrt{\frac{(2l+1)!}{4\pi}} \frac{e^{il\phi}}{2^l \cdot l!} \sin^l \theta$$

$$\therefore Y_{lm}(\theta, \phi) = \frac{1}{2^l l!} \sqrt{\frac{(2l+1)!}{4\pi}} \sqrt{\frac{1}{(2l)!} \frac{(l+m)!}{(l-m)!}} \left(\frac{L_-}{\hbar}\right)^{l-m} [e^{i\ell\phi} \sin^l \theta]$$

$$Y_{lm}(\theta, \phi) = \frac{1}{2^l l!} \sqrt{\frac{(2l+1) \cdot (l+m)!}{4\pi \cdot (l-m)!}} \left(\frac{L_-}{\hbar}\right)^{l-m} [e^{i\ell\phi} \sin^l \theta]$$

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

$$\langle \hat{x} | n, l, m \rangle = R_{nl}(r) Y_{lm}(\theta, \phi) \quad (V(\vec{r}) = V(r))$$

$$\langle r | n, l \rangle \langle \hat{n}(\theta, \phi) | l, m \rangle$$

Norm..  $\int_0^\infty dr \cdot r^2 |R_{nl}(r)|^2 = 1.$

$$\int d\Omega |Y_{lm}(\theta, \phi)|^2 = 1.$$

$$\int_{-1}^1 d\cos\theta \int_0^{2\pi} d\phi.$$

$l = \text{half integer}$  이면..

모든 방향에 대해  $l$  홀수 (정수  $\times$ )

$\therefore$  spherical harmonics 은

$l = \text{정수}$  일때만 존재!!