Tutorial # 12

№ 16.6.4

Stationary Schrödinger eq. in polar coordinates:

$$\begin{cases} \underbrace{-\frac{\hbar^2}{2m}\Delta\Psi + \overset{\text{potential}}{0}\cdot\Psi}_{=\hat{H}\Psi \text{ - Hamiltonian}} = E\Psi \Rightarrow -\left(\frac{1}{r}\cdot\frac{\partial}{\partial r}\left(r\cdot\frac{\partial\Psi}{\partial r}\right) + \frac{1}{r^2}\cdot\frac{\partial^2\Psi}{\partial\theta^2}\right) = \underbrace{\frac{2mE}{\hbar^2}}_{=:\mathcal{E}}\Psi \\ \Psi|_{r=a} = 0 \end{cases}$$

notation for brevity

$$\Psi(r,\theta) = R(r)\cdot Y(\theta)$$

$$\Rightarrow \frac{1}{r}(rR')'\cdot Y + \frac{1}{r^2}R\cdot Y'' = -\mathcal{E}RY$$

$$\cdot\frac{r^2}{YR} \Rightarrow \frac{r(rR')'}{R} + r^2\mathcal{E} = -\frac{Y''}{Y} = \lambda$$

$$Y'' + \lambda Y = 0 \Rightarrow Y(\theta) = C_1\cdot\cos(\sqrt{\lambda}\theta) + C_2\cdot\sin(\sqrt{\lambda}\theta)$$

$$Y(\theta + 2\pi) = Y(\theta) \Rightarrow \sqrt{\lambda} = n \Rightarrow \lambda_n = n^2, \quad n = 1, 2, \ldots$$

$$r^2R'' + rR' + (r^2\mathcal{E} - n^2)R = 0$$

$$\Rightarrow R(r) = A\cdot J_n(r\sqrt{\mathcal{E}}) + \underbrace{B\cdot Y_n(r\sqrt{\mathcal{E}})}_{=0 \text{ - from condition at } r=0}$$

$$R(a) = 0 \Rightarrow J_n(a\sqrt{\mathcal{E}}) = 0 \Rightarrow a\sqrt{\mathcal{E}} = \beta_{nk}$$

(k^{th} zero of J_n)

$$\Rightarrow a\sqrt{\frac{2mE}{\hbar^2}} = \beta_{nk} \Rightarrow$$

$$\Rightarrow E_{nm} = \frac{\hbar^2\beta_{nk}^2}{2ma^2}$$

- energy levels

N 16.6.9

$$\Delta\Psi = \frac{1}{r^2}\cdot\frac{\partial}{\partial r}\left(r^2\cdot\frac{\partial\Psi}{\partial r}\right) + \frac{1}{r^2\sin\theta}\cdot\frac{\partial}{\partial\theta}\left(\sin\theta\,\frac{\partial\Psi}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\cdot\frac{\partial^2\Psi}{\partial\varphi^2} = 0$$

$$\Psi(r,\theta,\varphi) = R(r)\cdot Y(\theta,\varphi)$$

$$\frac{1}{r^2}\left(r^2R'\right)'\cdot Y + \frac{R}{r^2}\cdot\frac{1}{\sin\theta}\cdot\frac{\partial}{\partial\theta}\left(\sin\theta\,\frac{\partial Y}{\partial\theta}\right) + \frac{R}{r^2\sin^2\theta}\cdot\frac{\partial^2 Y}{\partial\varphi^2} = 0$$

$$\underbrace{-\frac{\left(r^2R'\right)'}{R}}_{\text{function of } r} = \underbrace{\frac{1}{Y}\cdot\frac{1}{\sin\theta}\,\frac{\partial}{\partial\theta}\left(\sin\theta\,\frac{\partial Y}{\partial\theta}\right) + \frac{1}{Y}\cdot\frac{1}{\sin^2\theta}\,\frac{\partial^2 Y}{\partial\varphi^2}}_{\text{function of } \varphi,\,\theta} = \underbrace{-\lambda}_{\text{const}}$$

Let $\cos\theta =: x$. Then: $\frac{\partial}{\partial\theta} = \overbrace{\frac{\partial x}{\partial\theta}}^{=-\sin\theta}\cdot\frac{\partial}{\partial x}$

$$\frac{1}{Y}\underbrace{\sin\theta\cdot\frac{\partial}{\partial\theta}\left(\sin\theta\cdot\frac{\partial Y}{\partial\theta}\right)}_{=(1-x^2)\cdot\frac{\partial}{\partial x}\left((1-x^2)\frac{\partial Y}{\partial x}\right)} + \lambda\underbrace{\sin^2\theta}_{=1-x^2} = -\frac{1}{Y}\frac{\partial^2 Y}{\partial\varphi^2}$$

Separate further:

$$Y(\theta,\varphi) = X(\cos\theta)\cdot Z(\varphi)$$

$$\frac{(1-x^2)\left((1-x^2)\cdot X'\right)'}{X} + \lambda\cdot(1-x^2) = -\frac{Z''}{Z} = \mu$$

$$Z_1'' + \mu Z_1 = 0 \quad \Rightarrow \quad Z(\varphi) = A\cdot e^{i\sqrt{\mu}\varphi} + B\cdot e^{-i\sqrt{\mu}\varphi}$$

$$Z_1(\varphi) = Z_1(\varphi + 2\pi) \quad \Rightarrow \quad \sqrt{\mu} = m \Rightarrow \mu = m^2$$

$$Z_m(\varphi) = A_m \cdot e^{im\varphi}, \quad m \in \mathbb{Z}$$

may be negative so don't write the conjugated part

$$(1-x^2)\left[(1-x^2)\cdot X'\right]' + \lambda X\cdot(1-x^2) - \underbrace{\mu}_{= m^2}\cdot X = 0$$

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

it's equation for associated Legendre's polynomials

$$\Rightarrow X(x) =: P_\ell^{|m|}(x) = (1-x^2)^{|m|/2}\cdot\frac{d^{|m|}P_\ell}{dx^{|m|}} \quad \text{if} \quad \lambda = \ell(\ell+1), \ \ell \in \mathbb{Z}_+$$

Legendre's polynomial

$\Rightarrow (|m| \le \ell)$

$P_\ell^{|m|}(x)$

$$Y(\theta,\varphi) = \sum_{\ell=0}^{\infty}\sum_{|m|\le\ell} A_m \cdot \underbrace{P_\ell^{|m|}(\cos\theta)\cdot e^{im\varphi}}_{\sim\, Y_\ell^m(\theta,\varphi)}$$

spherical harmonic

N 16.6.18

$$-\frac{\hbar^2}{2m}\Delta\Psi = E\Psi \implies$$

$$\begin{cases} \Delta\Psi = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\Psi}{\partial r}\right) + \frac{1}{r^2\sin\theta}\cdot\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Psi}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\cdot\frac{\partial^2\Psi}{\partial\varphi^2} = -\underbrace{\frac{2mE}{\hbar^2}}_{=:\beta^2}\Psi \\ \Psi\big|_{r=a} = 0 \end{cases}$$

$$\Psi(r,\theta,\varphi) = R(r)\cdot Y(\theta,\varphi)$$

$$\implies \frac{\frac{\partial}{\partial r}\left(r^2 R'\right)}{R} + \frac{1}{Y\cdot\sin\theta}\cdot\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \frac{1}{Y\sin^2\theta}\cdot\frac{\partial^2 Y}{\partial\varphi^2} = -\beta^2 r^2$$

$$\overbrace{\frac{r^2R'' + 2rR'}{R} + \beta^2 r^2}^{\text{function of } r} = \overbrace{-\frac{1}{Y}\cdot\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial\varphi^2}\right]}^{\text{function of } \theta,\varphi}$$

$$= \lambda = l(l+1)$$

see N 16.6.9

$$r^2R'' + 2rR' + \left(\beta^2r^2 - l(l+1)\right)\cdot R = 0$$

$$R'' + \frac{2R'}{r} + \left(\beta^2 - \frac{l(l+1)}{r^2}\right)\cdot R = 0$$

Set $u(r) := R(r)\cdot\sqrt{r}$. Then: $R = \frac{u}{\sqrt{r}}$, $R' = \frac{1}{\sqrt{r}}\left(u' - \frac{u}{2r}\right)$

$$R'' = \frac{1}{\sqrt{r}}\left(u'' - \frac{u'}{2r}\right) - \frac{1}{2r\sqrt{r}}\left(u' - \frac{3u}{2r}\right)$$

$$= \frac{1}{\sqrt{r}}u'' - \frac{u'}{r\sqrt{r}} + \frac{3u}{4r^2\sqrt{r}}$$

$$u'' + \frac{2u'}{r} - \frac{u}{r^2} - \frac{u'}{r} + \frac{3u}{4r^2} + \left(\beta^2 - \frac{l(l+1)}{r^2}\right)u = 0$$

$$r^2u'' + ru' + \left(\beta^2r^2 - \underbrace{l(l+1) + \tfrac{1}{4}}_{=(l+\frac{1}{2})^2}\right)u = 0$$

$$u(r) = A\cdot J_{l+1/2}(\beta r) + B\cdot \underbrace{Y_{l+1/2}(\beta r)}_{\text{singular at } r=0 \implies B=0} \implies R_l(r) = \frac{A}{\sqrt{r}}\cdot J_{l+1/2}(\beta r)$$

$$R_\ell(r) = \frac{A}{\sqrt{r}} J_{\ell+1/2}(\beta r)$$

Recall BC:

k^{th} zero of $J_{\ell+1/2}$

$$\psi\Big|_{r=a} = 0 \Rightarrow J_{\ell+1/2}(\beta a) = 0 \Rightarrow \beta a = \gamma_{\ell k}$$

$$\frac{2mEa^2}{\hbar^2} = \gamma_{\ell k}^2$$

$$\Rightarrow E_{\ell k} = \frac{\hbar^2 \gamma_{\ell k}^2}{2ma^2}$$ – energy levels