L53-Angular Momentum Eigenfunctions

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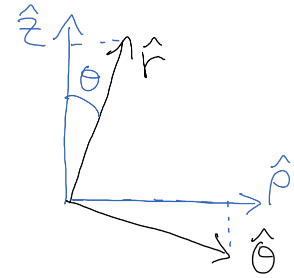
* co-ordinate representation of $\vec{L}, L^2$ operators

$$\vec{L} = \vec{r}\times\vec{p} = -i\hbar\,\vec{r}\times\nabla = -i\hbar(\hat{r}r)\times\left(\hat{r}\frac{\partial}{\partial r} + \hat{\theta}\frac{1}{r}\frac{\partial}{\partial\theta} + \hat{\phi}\frac{1}{r\sin\theta}\frac{\partial}{\partial\phi}\right)$$

$$= -i\hbar\left(\hat{\phi}\frac{\partial}{\partial\theta} - \hat{\theta}\frac{1}{\sin\theta}\frac{\partial}{\partial\phi}\right)$$

$$(\hat{r}\ \hat{\theta}\ \hat{\phi}) = (\hat{x}\ \hat{y}\ \hat{z})\begin{pmatrix} s_\theta c_\phi & c_\theta c_\phi & -s_\phi \\ s_\theta s_\phi & c_\theta s_\phi & c_\phi \\ c_\theta & -s_\theta & 0 \end{pmatrix}$$



$$\vec{L} = -i\hbar\left((-\hat{x}s_\phi + \hat{y}c_\phi)\frac{\partial}{\partial\theta} - (\hat{x}c_\theta c_\phi + \hat{y}c_\theta s_\phi - \hat{z}s_\theta)\frac{1}{s_\theta}\frac{\partial}{\partial\phi}\right)$$

$$L_x = -i\hbar\left(-s_\phi\frac{\partial}{\partial\theta} - c_\phi\cot\theta\frac{\partial}{\partial\phi}\right)$$

$$L_y = -i\hbar\left(c_\phi\frac{\partial}{\partial\theta} - s_\phi\cot\theta\frac{\partial}{\partial\phi}\right)$$

$$L_z = -i\hbar\frac{\partial}{\partial\phi}$$

note: $\frac{\partial}{\partial\phi}$ also in L_x, L_y.

$$L_\pm = L_x \pm iL_y = \hbar\left(\underbrace{(is_\phi \pm c_\phi)}_{\pm(c_\phi \pm is_\phi)}\frac{\partial}{\partial\theta} + i(c_\phi \pm is_\phi)\cot\theta\frac{\partial}{\partial\phi}\right)$$

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

$$L_\pm L_\mp = \pm\hbar e^{\pm i\phi}\left(\frac{\partial}{\partial\theta} \pm i\cot\theta\frac{\partial}{\partial\phi}\right)\cdot\mp\hbar e^{\mp i\phi}\left(\frac{\partial}{\partial\theta} \mp i\cot\theta\frac{\partial}{\partial\phi}\right)$$ [Prob # 4.21]

$$= -\hbar^2\left(\frac{\partial^2}{\partial\theta^2} \mp i\underbrace{\left(-\csc^2\theta + \cancel{\cot\theta\frac{\partial}{\partial\theta}}\right)}_{\frac{\partial}{\partial\theta}\cot\theta\ldots}\frac{\partial}{\partial\phi} \pm i\cot\theta\underbrace{e^{\pm i\phi}\frac{\partial}{\partial\phi}e^{\mp i\phi}}_{\mp i + \cancel{\frac{\partial}{\partial\phi}}}\frac{\partial}{\partial\theta} + \cot^2\theta\cdot\underbrace{e^{\pm i\phi}\frac{\partial}{\partial\phi}e^{\mp i\phi}}_{\mp i + \frac{\partial}{\partial\phi}}\frac{\partial}{\partial\phi}\right)$$

$$= -\hbar^2\left(\frac{\partial^2}{\partial\theta^2} + \cot\theta\frac{\partial}{\partial\theta} \pm i\overbrace{(\csc^2\theta - \cot^2\theta)}^{1}\frac{\partial}{\partial\phi} + \cot^2\theta\frac{\partial^2}{\partial\phi^2}\right)$$

$$= -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{\cos^2\theta}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right] \pm \underbrace{\hbar\cdot -i\hbar\frac{\partial}{\partial\phi}}_{\hbar L_z = \frac{1}{2}[L_+, L_-]}$$

$$= L_x^2 + L_y^2 \pm \hbar L_z$$

$$L^2 = (L_+L_- - \hbar L_z) + L_z^2 = -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]$$

* top rung eigenfunction [Prob#4.22]

$$\langle \Omega | L_+ | \ell\ell \rangle = \hbar e^{i\phi}\left(\frac{\partial}{\partial\theta} + i\cot\theta \frac{\partial}{\partial\phi}\right) Y_{\ell\ell}(\theta,\phi) = 0$$

let $Y_{\ell\ell} = f(\theta)\cdot e^{i\ell\phi}$ so that $L_z e^{i\ell\phi} = -i\hbar\partial_\phi e^{i\ell\phi} = \hbar\ell e^{i\ell\phi}$

$$\frac{df}{d\theta} - \ell\cot\theta\cdot f = 0 \qquad \frac{df}{f} = \ell\frac{\cos\theta\, d\theta}{\sin\theta} = \ell\frac{d\sin\theta}{\sin\theta}$$

$$\ln f = \ln(\sin\theta)^\ell \qquad f(\theta) = \sin^\ell\theta$$

thus $Y_{\ell\ell}(\theta,\phi) = N\sin^\ell\theta\, e^{i\ell\phi}$

$$\langle \ell\ell|\ell\ell\rangle = \int d\Omega\, Y^*_{\ell\ell}(\theta,\phi)Y_{\ell\ell}(\theta,\phi) = |N|^2\int_0^\pi \sin\theta\, d\theta\int_0^{2\pi} d\phi\, \sin^{2\ell}\theta\, \cancel{e^{i(\ell-\ell)\phi}} = 2\pi|N|^2 I_\ell = 1$$

where $I_\ell = \int_0^\pi \sin^{2\ell+1}\theta\, d\theta = \int_0^\pi \underbrace{\sin^{2\ell}\theta}_{u}\cdot d\underbrace{(-\cos\theta)}_{v}$

$$= \overset{0}{\cancel{-\sin^{2\ell}\theta\cdot\cos\theta\Big|_0^\pi}} + \int_0^\pi \cos\theta\, d(\sin^{2\ell}\theta)$$

$$= \int_0^\pi 2\ell\cdot\sin^{2\ell-1}\theta\cdot\underbrace{\cos^2\theta}_{1-\sin^2\theta}\, d\theta = 2\ell\,(I_{\ell-1} - I_\ell)$$

thus $I_\ell = \frac{2\ell}{2\ell+1}I_{\ell-1} = \frac{2\cdot4\cdot\cdots(2\ell)}{3\cdot5\cdot\cdots(2\ell+1)}I_0$; $I_0 = \int_0^\pi \sin\theta\, d\theta = 2$

$$|N|^2 = \frac{1}{2\pi I_\ell} = \frac{1}{4\pi}\,\frac{1}{\frac{2}{1}\cdot\frac{4}{3}\cdot\frac{6}{5}\cdot\frac{2\ell}{7}\cdots\frac{}{2\ell+1}} = \frac{1}{4\pi}\,\frac{2^2\cdot4^2\cdots(2\ell)^2}{1\cdot2\cdot3\cdot4\cdots2\ell+1} = \frac{(2^\ell\ell!)^2}{4\pi(2\ell+1)!}$$

$$\boxed{Y_{\ell\ell}(\theta,\phi) = \frac{2^\ell\ell!}{\sqrt{4\pi(2\ell+1)!}}\underbrace{\sin^\ell\theta\, e^{i\ell\phi}}_{\sin\theta(\cos\phi+i\sin\phi) = \left(\frac{x+iy}{\rho}\right)^\ell}}$$ up to an arbitrary phase $\equiv 1$

* lower rungs: use $L_\pm|\ell m\rangle = \hbar\sqrt{(\ell\mp m)(\ell\pm m+1)}\,|\ell, m\pm1\rangle$

  - apply L_- repeatedly to $Y_{\ell\ell}$ to get all $Y_{\ell m}$ for ℓ.

$$\boxed{Y_{\ell m}(\theta,\phi) = (-1)^m\sqrt{\frac{2\ell+1}{4\pi}\frac{(\ell-m)!}{(\ell+m)!}}\,P_\ell^m(\cos\theta)\,e^{im\phi}}$$

$$L_\pm[Y_{\ell m}] = \pm\hbar e^{\pm i\phi}\left(\frac{\partial}{\partial\theta} \pm i\cot\theta\frac{\partial}{\partial\phi}\right)\left[(-1)^m\sqrt{\frac{2\ell+1}{4\pi}\frac{(\ell-m)!}{(\ell+m)!}}\,P_\ell^m e^{im\phi}\right]$$

$$= \hbar\sqrt{(\ell \mp m)(\ell \pm m+1)} \cdot \left[(-1)^{m\pm1}\sqrt{\frac{2\ell+1}{4\pi}\frac{(\ell-m\mp1)!}{(\ell+m\pm1)!}}\, P_\ell^{m\pm1} e^{i(m\pm1)\phi}\right]$$

– use this equation to construct recurrence relations for P_ℓ^m

$$\left[\frac{d}{d\xi}(1-\xi^2)\frac{d}{d\xi} - \frac{m^2}{1-\xi^2} + \ell(\ell+1)\right] P_\ell^m(\xi) = 0 \qquad \text{Sturm-Liouville ODE}$$

$$P_\ell^m(\xi) = \underbrace{(1-\xi^2)^{m/2}}_{\sin^m\theta}\left(\frac{d}{d\xi}\right)^m P_\ell(\underbrace{\xi}_{\cos\theta}) \qquad \text{where} \qquad P_\ell(\xi) = \frac{1}{2^\ell \ell!}\left(\frac{d}{d\xi}\right)^\ell(\xi^2-1)^\ell$$

$$\frac{dP}{d\xi} = \frac{d}{d\xi}\left[(1-\xi^2)^{m/2}\left(\frac{d}{d\xi}\right)^m P_\ell(\xi)\right]$$

$$= \frac{m}{2}(1-\xi^2)^{m/2-1}(-2\xi)\,\frac{d}{d\xi}^m P_\ell(\xi) + (1-\xi^2)^{m/2}\left(\frac{d}{d\xi}\right)^{m+1} P_\ell(\xi)$$

$$= \frac{1}{\sqrt{1-\xi^2}} P_\ell^{m+1} - \frac{m\xi}{1-\xi^2} P_\ell^m$$

– use $L_\pm = L_x \pm iL_y$ to calculate $L_x|\ell m\rangle$ or $L_y|\ell m\rangle$

* summary: we use H, L^2, L_z as a C.S.C.O (Complete set of Commuting Operators) to completely characterize the eigenfunctions of Hamiltonians with rotational symmetry (eg. central potentials like H-atom, 3-d oscillator, ...)

$$\mathcal{H} = \frac{p^2}{2m} + V = -\frac{\hbar^2}{2m}\nabla^2 + V = -\hbar^2\frac{1}{r}\frac{\partial^2}{\partial r^2}r + \underbrace{\frac{L^2}{2I}}_{-\hbar^2\ell(\ell+1)} + V(r)$$

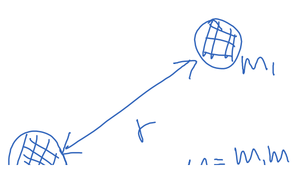
centripetal potential.

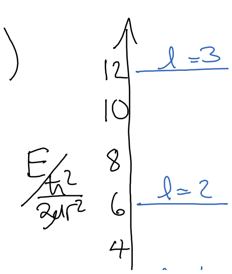
Energy is degenerate in "m"

$$\psi(r,\theta,\phi) = R(r)\,Y_{\ell m}(\theta,\phi) \qquad L^2 Y_{\ell m} = \hbar^2 \ell(\ell+1)\, Y_{\ell m}$$
$$L_z Y_{\ell m} = \hbar m\, Y_{\ell m}$$

* Example: diatomic molecule: (rigid rotor)

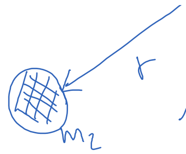
if r is fixed then





$$\mathcal{H} = \frac{L^2}{\ } = \frac{\hbar^2\ell(\ell+1)}{\ }$$

$$\mathcal{H} = \frac{L^2}{2I} = \frac{\hbar^2 \ell(\ell+1)}{2\mu r^2}$$



$$\mu = \frac{m_1 m_2}{m_1 + m_2}$$