# L28-Angular Momentum and Spherical Square Well

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$\ast$ Angular Momentum – recall 3 nested S.-L. problems

$$\hat{T} = \frac{\hat{p}^2}{2m} = \frac{-\hbar^2}{2m}\nabla^2 = \frac{-\hbar^2}{2m}\cdot\frac{1}{r^2}\left(\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} + \frac{1}{\sin\theta}\left(\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin\theta}\frac{\partial^2}{\partial\phi^2}\right)\right)$$

$$= \underbrace{\left(-\hbar^2\cdot\frac{1}{r}\frac{\partial^2}{\partial r^2}r\right)/2m}_{\hat{T}_r = \hat{P}_r^2/2m} + \left[\underbrace{\frac{-\hbar^2}{\sin\theta}\left(\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta}\right)}_{\hat{L}_\theta^2} + \frac{1}{\sin^2\theta}\underbrace{\left(-\hbar^2\frac{\partial^2}{\partial\phi^2}\right)}_{\hat{L}_\phi^2}\right]/\underbrace{2mr^2}_{I}$$

$\hat{T}_\Omega = \hat{L}^2/2I$

$\hat{L}_z = -i\hbar\partial_\phi \qquad \hat{L}_z e^{im\phi} = \hbar m\, e^{im\phi}$

periodic boundary conditions: $\Phi(0) = \Phi(2\pi) \qquad \Phi'(0) = \Phi'(2\pi)$

$\Rightarrow m = 0, \pm1, \pm2, \ldots \in \mathbb{Z}$

$$\hat{L}^2 = \hbar^2\cdot\frac{-1}{\sin\theta}\left(\frac{\partial}{\partial\theta}\frac{\sin^2\theta}{\sin\theta}\frac{\partial}{\partial\theta} - \frac{m^2}{\sin\theta}\right) \qquad L^2\,\Theta(\theta) = \hbar^2 \ell(\ell+1)\,\Theta(\theta)$$

let $x = \cos\theta = c_\theta$

$dx = -\sin\theta\, d\theta$

$\sqrt{1-x} = \sin\theta = s_\theta$

$$= \hbar^2\left(\frac{-d}{dx}(1-x^2)\frac{d}{dx} + \frac{m^2}{1-x^2}\right)$$

$$\hat{L}^2 P_\ell^{|m|}(x) = \hbar^2\ell(\ell+1)\underbrace{P_\ell^{|m|}(x)}$$ Associated Legendre functions

if $m=0$ (azimuthal symmetry, $L_z=0$) $\quad P_\ell^{|m|}(x) \to P_\ell(x)$ Legendre polynomial

$$P_\ell(x) \equiv \frac{1}{2^\ell \ell!}\left(\frac{d}{dx}\right)^\ell (x^2-1)^\ell$$ Rodriguez formula

if $m>0 \quad P_\ell^m(x) \equiv \underbrace{(1-x^2)^{|m|/2}}_{s_\theta^{|m|}}\left(\frac{d}{dx}\right)^{|m|} P_\ell(x)$

$m=0$: $\ell = 0,1,2\ldots$

$P_0(x) = 1$

$P_1(x) = x = c_\theta$

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

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

$|m|=1$: $\ell = 1,2,3\ldots$

$P_1^1(x) = -s_\theta$

$P_2^1(x) = -3c_\theta s_\theta$

$P_3^1(x) = -3/2(5c_\theta^2 - 1)s_\theta$

$|m|=2$: $\ell = 2,3,\ldots$

$P_2^2(x) = 3s_\theta^2$

$P_3^2(x) = 15c_\theta s_\theta^2$

$|m|=3 \quad \ell = 3,4,\ldots$

$P_3^3(x) = -15s_\theta^3$

* Application: solution of $\nabla^2 V = 0$ in spherical co-ords:

$$\left[\frac{1}{r}\frac{\partial^2}{\partial r^2} r - \ell(\ell+1)\right] R(r) = 0 \qquad \text{let } u(r) = rR(r)$$

$$u'' = \ell(\ell+1)u \qquad u = e^{\pm\sqrt{\ell(\ell+1)}\,r} \quad \text{or} \quad u = \underbrace{r^{\ell+1}}_{\text{nonsingular at } r\to 0} \text{ or } r^{-\ell}$$

$$V(r,\theta,\phi) = \sum_{\ell m} r^\ell P_\ell^{|m|}(c_\theta)\, e^{im\phi}$$

$$= \sum_{\ell m} r^{\ell-|m|}\left(a\, c_\theta^{\ell-|m|} + b\, c_\theta^{\ell-|m|-2} + \dots\right) r^{|m|} s_\theta^{|m|} (c_\phi + i s_\phi)^m$$

$$= \sum_{\ell m} \left(a z^{\ell-|m|} + b z^{\ell-|m|-2} r^2 + \dots\right)(x \pm iy)^m$$

$$= \sum_{\substack{i+j=|m| \\ i+j+k=\ell \\ i,j,k \geq 0}} a_{ijk}\, x^i y^j z^k \qquad \text{multinomial in } x,y,z! \text{ (but not all)}$$

$$\nabla^2 V = \sum_{ijk} a_{i'j'k'}(\partial_x^2 + \partial_y^2 + \partial_z^2)\, x^{i'} y^{j'} z^{k'}$$

$$= \sum_{ijk} a_{i'j'k'}\left[i'(i'-1)x^{i'-2} y' z' + \dots\right] = \sum_{ijk} \underbrace{\begin{pmatrix} +\, i{+}2 \cdot i{+}1 \cdot a_{i+2\,jk} \\ j{+}2 \cdot j{+}1 \cdot a_{i\,j+2\,k} \\ +\, k{+}2 \cdot k{+}1 \cdot a_{ijk+2} \end{pmatrix}}_{=0 \ \forall i,j,k} x^i y^j z^k$$

Example: $a_{200} + a_{020} + a_{002} = 0$ excludes $\ell=0$. $r^2 = x^2+y^2+z^2$, but holds for

$\ell=2$: [ $m=2$: $x^2-y^2$, $2xy$, $m=1$: $2xz$, $2yz$, $m=0$: $\frac{1}{2}(3z^2-r^2)$ ]

$|m|=0$: s = sharp ($\ell=0$) p = princi pal ($\ell=1$) d = diffuse ($\ell=3$) f = fine ($\ell=4$)

$\ell=0$ $\quad s = 1$ $\qquad$ $|m|=1$:

$1$ $\quad p_z = z$ $\qquad p_x = x \quad p_y = y$ $\qquad |m|=2$:

$2$ $\quad d_{3z^2-r^2} = z^2 - \frac{1}{2}(x^2+y^2)$ $\qquad d_{xz} = 2xz \quad d_{yz} = 2yz$ $\qquad d_{xy} = 2xy \quad d_{x^2-y^2} = x^2-y^2$

$3$ $\quad f_{5z^3-3r^2z} = z^3 - \frac{3}{2}(x^2+y^2)z$ $\qquad f_{5z^2x-r^2x} = 6z^2x - \frac{3}{2}(x^3+xy^2)$ $\qquad f_{xyz} = 30\,xyz$

$\qquad f_{5z^2y-r^2y} = 6z^2y - \frac{3}{2}(y^3+yx^2)$ $\qquad f_{x^2z-y^2z} = 15(x^2z - y^2z)$

$|m|=3$: $f_{x^3-3xy^2} = 15(x^3-3xy^2)$, $f_{y^3-3yx^2} = 15(y^3-3yx^2)$

* spherical harmonics (angular eigenfunctions)

– need to normalize: $\langle e^{im\phi} | e^{im'\phi} \rangle = \int_0^{2\pi} d\phi \, e^{-i(m-m')\phi} = 2\pi \, \delta_{mm'}$

$\langle P_\ell | P_{\ell'} \rangle = \int_{-1}^{1} dx \, P_\ell(x) P_{\ell'}(x) = \frac{2}{2\ell+1} \delta_{\ell\ell'} \quad \Rightarrow \quad \langle P_\ell^{|m|} | P_{\ell'}^{|m|} \rangle = \frac{2}{2\ell+1} \frac{(\ell+|m|)!}{(\ell-|m|)!} \delta_{\ell\ell'}$

– thus $Y_{\ell m}(\theta,\phi) \equiv \varepsilon \sqrt{\frac{2\ell+1}{4\pi} \frac{(\ell-|m|)!}{(\ell+|m|)!}} \, P_\ell^{|m|}(\cos\theta) \, e^{im\phi}$

so that $\boxed{\langle \ell m | \ell' m' \rangle = \delta_{\ell\ell'} \delta_{mm'}} \equiv \int_{\theta=0}^{\pi} \int_{\phi=0}^{2\pi} \underbrace{\sin\theta \, d\theta \, d\phi}_{d\Omega} \, Y_{\ell m}^*(\theta,\phi) \, Y_{\ell' m'}(\theta,\phi)$

closure: $\boxed{\sum_{\ell m} |\ell m\rangle\langle \ell m| = I} \qquad \sum_{\ell m} Y_{\ell m}(\theta,\phi) Y_{\ell m}(\theta',\phi') = \delta(c_\theta - c_{\theta'}) \delta(\phi-\phi')$

* application: spherical "square" well (Helmholtz Eq.)

$$\hat{H} \Psi(\vec{r}) = \frac{-\hbar^2}{2m} \nabla^2 \Psi(\vec{r}) = \left[ \frac{-\hbar^2}{2m} \frac{1}{r} \frac{\partial^2}{\partial r^2} r + \frac{\hat{L}^2}{2mr^2} \right] \Psi(\vec{r}) = E \Psi(\vec{r})$$

let $\Psi(\vec{r}) = R(r) \cdot Y_{\ell m}(\Omega) \qquad u(r) \equiv r R(r) \qquad E = \frac{\hbar^2 k^2}{2m}$

$\left( \frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2} \right) u = -k^2 u$ "spherical Bessel equation"

$u(r) = j_\ell(kr)$ "spherical Bessel function"

Boundary conditions: at $r \to 0$, ignore $\cancel{n_\ell(kr)}$

at $r = a$, $j_\ell(ka) = 0 \Rightarrow k_n a = x_{n\ell}$ "$n^{th}$ zero of $j_\ell(x)$"