General Sturm-Liouville problem

$$\frac{d}{dx}\left(f(x)y'\right) - g(x)y + \lambda w(x)\, y = 0$$

Solutions : complete set of orthogonal functions y_λ

$$\int_a^b y_\lambda \cdot y_{\lambda'} \cdot w(x)\, dx = 0 \quad \text{for } \lambda \neq \lambda'$$

In particular, if the equation can be written as

$$\frac{d}{dx}\left[\alpha(x) w(x) y'\right] + \lambda w(x) y = 0$$

then the solutions are orthogonal polynomials, that can be calculated using Rodrigues formula:

$$y_n(x) = \mathcal{N} \frac{1}{w(x)} \frac{d^n}{dx^n}\left(w(x)\left[\alpha(x)\right]^n\right)$$

$$\boxed{\frac{d}{dx}\left[(1-x^2)y'\right] + \ell(\ell+1)y = 0 \Rightarrow P_\ell(x) = \frac{1}{2^\ell \ell!} \frac{d^\ell}{dx^\ell}(x^2-1)^\ell}$$

Also, many polynomials can be reproduce using a corresponding generation function: $\Phi(x,h) = \sum_{n=0}^{\infty} C_n y_n(x)\, h^n$

Example of the polynomials:

Hermite polynomials: $y'' - 2xy' + 2ny = 0 \Rightarrow \frac{d}{dx}\left(e^{-x^2} y'\right) + 2ne^{-x^2} y$

here $\alpha(x) = 1$, $w(x) = e^{-x^2}$

Rodrigues formula : $H_n = (-1)^n e^{x^2} \frac{d^n}{dx^n} e^{-x^2}$

Generation function : $\Phi(x,h) = e^{2xh-h^2} = \sum_{n=0}^{\infty} H_n(x) \frac{h^n}{n!}$

Orthogonality: $\int_{-\infty}^{\infty} e^{-x^2} H_n(x) H_m(x)\, dx = \sqrt{\pi}\, 2^n \cdot n!\, \delta_{nm}$

Laguerre polynomials: $xy'' + (1-x)y' + ny = 0 \Rightarrow \frac{d}{dx}\left[xe^{-x} y'\right] + ne^{-x} y = 0$

here $\alpha(x) = x$, $w(x) = e^{-x}$; Rodrigues formula: $L_n(x) = \frac{1}{n!} e^x \frac{d^n}{dx^n}(x^n e^{-x})$

Generation function: $\Phi(x,h) = \dfrac{e^{-\frac{xh}{1-h}}}{1-h} = \sum_{n=0}^{\infty} L_n(x)\, h^n$

Orthogonality: $\int_0^{\infty} e^{-x} L_n(x) L_m(x)\, dx = \delta_{nm}$

Bessel functions:

$$x^2y'' + xy' + (x^2 - p^2)y = 0 \quad \Rightarrow \quad \frac{1}{x}\frac{d}{dx}(xy') + \left(1 - \frac{p^2}{x^2}\right)y = 0$$

Solutions $J_p(x) \rightarrow$ set of orthogonal functions.

Associate Legendre polynomials:

$$(1-x^2)y'' - 2xy + \left(\ell(\ell+1) - \frac{m^2}{1-x^2}\right)y = 0 \Rightarrow \frac{d}{dx}\left((1-x^2)y'\right) + \left[\ell(\ell+1) - \frac{m^2}{1-x^2}\right]y = 0$$

or, using $x = \cos\theta$

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\left[\sin\theta\, y'\right] + \left[\ell(\ell+1) - \frac{m^2}{\sin^2\theta}\right]y = 0$$

Solutions: $P_\ell^m(x)$ or $P_\ell^m(\theta) \rightarrow$ associate Legendre functions

(not all $P_\ell^m(x)$ are polynomials)

$$P_\ell^m(x) = (1-x^2)^{m/2}\frac{d^m}{dx^m}P_\ell(x)$$

$\rightarrow$ but this expression works only for positive m

In general, we will have to use Rodrigues formular for $P_\ell^m(x)$:

$$P_\ell^m(x) = (1-x^2)^{m/2}\frac{1}{2^\ell \ell!}\frac{d^{\ell+m}}{dx^{\ell+m}}(x^2-1)^\ell$$

Because of the definition P_ℓ^m and P_ℓ^{-m}

$$P_\ell^m(x) = (-1)^m\frac{(\ell+m)!}{(\ell-m)!}P_\ell^{-m}(x)$$

Orthogonality: associate Legendre functions of the same argument m are orthogonal:

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

Examples: let's calculate a few first ass. Legendre func:

$P_\ell^0(x) = P_\ell(x)$ $\qquad P_0(x) = 1, \quad P_1(x) = x, \quad P_2(x) = \frac{3}{2}x^2 - \frac{1}{2}$

$P_0^0(x) = 1$

$P_1^0(x) = x \quad [\cos\theta] \qquad P_1^1(x) = \sqrt{1-x^2}\,\frac{1}{2}\frac{d^2}{dx^2}(x^2-1) = \sqrt{1-x^2} = [\sin\theta]$

$$P_1^{-1}(x) = \frac{1}{\sqrt{1-x^2}}\frac{1}{2}(x^2-1) = -\frac{1}{2}\sqrt{1-x^2} = \left[-\frac{1}{2}\sin\theta\right]$$

Two "special cases"

$m=\ell$ $$P_\ell^\ell = (1-x^2)^{\ell/2}\frac{1}{2^\ell \ell!}\frac{d^{2\ell}}{dx^{2\ell}}\overset{x^{2\ell}+\dots}{(x^2-1)^\ell} = (1-x^2)^{\ell/2}\frac{(2\ell)!}{2^\ell\cdot\ell!} = \left[\frac{(2\ell)!}{2^\ell\ell!}(\sin\theta)^\ell\right]$$

$m=-\ell$ $$P_\ell^{-1} = (1-x^2)^{\ell/2}\frac{1}{2^\ell\ell!}(x^2-1)^\ell = \frac{(-1)^\ell}{2^\ell\ell!}(1-x^2)^{\ell/2} = \left[\frac{(-1)^\ell}{2^\ell\ell!}(\sin\theta)^\ell\right]$$

Associate Legendre functions are essencial components of <u>spherical functions</u> (or spherical harmonics)

Many major physics equations involve $\nabla^2 F(\vec{r}) = \left(\frac{\partial^2 F}{\partial x^2} + \frac{\partial^2 F}{\partial y^2} + \frac{\partial^2 F}{\partial z^2}\right)$

In spherical coordinates this operator is:

$$\left[\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right]F(r,\theta,\varphi) + \frac{1}{r^2}\left\{\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial F}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2 F}{\partial\varphi^2}\right\}$$

If one solves an equation $\nabla^2 F = 0$ or $\nabla^2 F = f(r)F$

all angular-dependent terms are inside $\{\ldots\}$

So we can separate the variables and search

for $F(r,\theta,\varphi) = R(r)\,Y(\theta,\varphi)$

Then (for the sake of argument I will use $\nabla^2 F = 0$ — Laplas equ)

$$\frac{1}{YR}\quad Y(\theta,\varphi)\left[R'' + \frac{2}{r}R'\right] + \frac{R}{r^2}\underbrace{\left\{\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial Y}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial\varphi^2}\right\}}_{=\text{const} = -\ell(\ell+1)} = 0$$

Then the equation for the spherical part

$$\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial Y}{\partial\theta}+\frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial\varphi^2}+\ell(\ell+1)Y=0$$

If we separate variables again: $Y(\theta,\varphi)=P(\theta)\Phi(\varphi)$

$$\Phi\frac{1}{\sin\theta}\frac{d}{d\theta}\left[\sin\theta P'(\theta)\right]+\frac{P(\theta)}{\sin^2\theta}\Phi''+\ell(\ell+1)P\cdot\Phi=0 \quad \times\frac{1}{P\cdot\Phi}$$

$$\frac{1}{P}\frac{1}{\sin\theta}\frac{d}{d\theta}\left[\sin\theta P'(\theta)\right]+\frac{1}{\sin^2\theta}\underbrace{\left\{\frac{\Phi''}{\Phi}\right\}}_{=\text{const}\,=\,-m^2}+\ell(\ell+1)=0$$

Azimuthal ~~pafot~~ part $\Phi''=-m^2\Phi \Rightarrow \Phi=\left\{\begin{matrix}\cos m\varphi\\ \sin m\varphi\end{matrix}\right\}=e^{\pm im\varphi}$

Can we say anything about values of m?

In physical world $\varphi,\ \varphi+2\pi,\ \varphi+4\pi$ correspond to the same point in space, so it is reasonable to request that $\Phi(\varphi)=\Phi(\varphi+2\pi) \Rightarrow e^{im\varphi}=e^{im(\varphi+2\pi)}$

$\Rightarrow m$ should be integer

Back to the equation for "θ"

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\left[\sin\theta P'(\theta)\right]-\frac{m^2}{\sin^2\theta}P(\theta)+\ell(\ell+1)P(\theta)=0$$

solutions $\Rightarrow$ associate Legendre functions $P_\ell^m(\theta)$

Thus: $Y(\theta,\varphi)=Y_{\ell,m}(\theta,\varphi)=A_{\ell m}\,P_\ell^m(\theta)\,\Phi_m(\varphi)$

Orthogonality: we want to request that $Y_{\ell m}(\theta,\varphi)$ are <u>orthonormal</u>: $\int_0^\pi\sin\theta\,d\theta\int_0^{2\pi}d\varphi\;Y_{\ell m}\cdot Y^*_{\ell'm'}=\delta_{\ell\ell'}\delta_{mm'}$

That means that:

$$A_{\ell m}A^*_{\ell'm'}\underbrace{\left(\int_0^{2\pi}e^{im\varphi}\cdot e^{-im'\varphi}d\varphi\right)}_{=2\pi\delta_{mm'}}\left(\int_0^\pi P_\ell^m P_{\ell'}^{m'}\sin\theta\,d\theta\right)=\delta_{\ell\ell'}\delta_{mm'}$$

$$\frac{1}{2\pi}\int_0^{2\pi}e^{i(m-m')\varphi}d\varphi=\delta_{mm'}$$

$$2\pi A_{\ell m}A_{\ell'm}\delta_{mm'}\int_{-1}^{1}P_\ell^m(x)P_{\ell'}^m(x)\,dx=\delta_{\ell\ell'} \qquad x=\cos\theta$$

$$2\pi \, |A_{\ell m}|^2 \, \delta_{mm'} \frac{2}{2\ell+1} \frac{(\ell+m)!}{(\ell-m)!} \delta_{\ell\ell'} = \delta_{mm'} \delta_{\ell\ell'}$$

$$\Rightarrow A_{\ell m} = \sqrt{\frac{2\ell+1}{4\pi} \frac{(\ell-m)!}{(\ell+m)!}} \cdot (-1)^m$$

Thus: Spherical harmonics $\underline{Y_{\ell m} = (-1)^m \sqrt{\frac{2\ell+1}{4\pi} \frac{(\ell-m)!}{(\ell+m)!}} P_\ell^m(\cos\theta) e^{im\varphi}}$

First few spherical functions:

$\ell=m=0$ $\quad Y_{00}(\theta,\varphi) = \frac{1}{\sqrt{4\pi}} \quad (\ell=0, m=0)$

$\ell=1, m=0 \quad Y_{10} = \sqrt{\frac{3}{4\pi}} \cos\theta$

$\ell=1, m=1 \quad Y_{11} = (-1)^1 \sqrt{\frac{3}{4\pi} \cdot \frac{1}{2}} \sin\theta \, e^{i\varphi} = -\sqrt{\frac{3}{8\pi}} \sin\theta \, e^{i\varphi}$

$\ell=1, m=-1 \quad Y_{1,-1} = (-1)^{-1} \sqrt{\frac{3}{4\pi} \cdot 2} \cdot \left(-\frac{1}{2} \sin\theta\right) e^{-i\varphi} = \sqrt{\frac{3}{8\pi}} \sin\theta \, e^{i\varphi}$

Physical meaning

Spherical harmonics are the eigenvalues of angular momentum operator in QM

$\vec{L} = \vec{r} \times \vec{p}$ (in classical physics)

In quantum mechanics $\hat{\vec{L}}$ becomes an operator: $\hat{\vec{L}} = -i\hbar(r \times \nabla)$ $\{\hat{L}_x, \hat{L}_y, \hat{L}_z\}$ do not commute (i.e they cannot be measured simultaneously). Important operators are: $\hat{L}^2 = (\vec{L} \cdot \vec{L})$, and $\hat{L}_z$ — z-component of $\vec{L}$

In spherical coordinates

$$\hat{L}^2 = -\frac{\hbar^2}{\sin\theta} \frac{\partial}{\partial\theta}\left(\sin \frac{\partial}{\partial\theta}\right) - \frac{\hbar^2}{\sin^2\theta} \frac{\partial^2}{\partial\varphi^2}$$

and

$$\vec{L}_z = -i\hbar \frac{\partial}{\partial\varphi}$$

It is easy to see that $\Phi_m(\varphi) = \frac{1}{\sqrt{2\pi}} e^{im\varphi}$ are the eigen functions of $\hat{\vec{L}}_z$

$$\hat{\vec{L}}_z \Phi_m(z) = -i\hbar \frac{\partial}{\partial\varphi}\left(\frac{1}{\sqrt{2\pi}} e^{im\varphi}\right) = \frac{1}{\sqrt{2\pi}} \hbar m\, e^{im\varphi} = \underline{\hbar m}\, \Phi_m(\varphi)$$

and $Y_{\ell m}(\theta,\varphi)$ are the eigen functions of $\hat{\vec{L}}^2$

$$\hat{\vec{L}}^2 Y_{\ell m}(\theta,\varphi) = -\hbar^2 \left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right) Y_{\ell m}(\theta,\varphi) = \underline{\hbar^2 \ell(\ell+1)}\, Y_{\ell m}(\theta,\varphi)$$

Thus, if the state of the system is described by a particular spherical harmonics $Y_{\ell m}(\theta,\varphi)$ then its (squared) total angular momentum $\langle \hat{L}^2 \rangle = \hbar^2 \ell(\ell+1)$, and its z-component $\langle L_z \rangle = m$