L27-Curvilinear Laplacian Eigenfunctions

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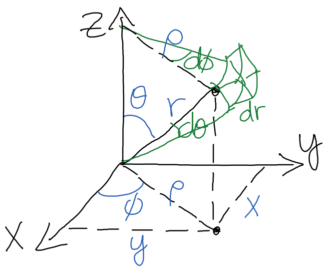
* Curvilinear coordinates

cart	cyl	sph
x	$= \rho c_\phi$	$= r s_\theta c_\phi$
y	$= \rho s_\phi$	$= r s_\theta s_\phi$
z	$= z$	$= r c_\theta$
	ρ	$= r s_\theta$



$$d\tau = dx\, dy\, dz \quad \text{[cart]}$$
$$= d\rho \cdot \rho d\phi \cdot dz \quad \text{[cyl]}$$
$$= dr \cdot r d\theta \cdot \rho d\phi \quad \text{[sph]}$$
$$= \underset{\sim}{h_1} dq^1 \cdot \underset{\sim}{h_2} dq^2 \cdot \underset{\sim}{h_3} dq^3$$

$$\nabla^2 = \underbrace{\frac{1}{h_1 h_2 h_3}}_{d\tau} \sum_i \frac{\partial}{\partial q^i} \underbrace{\frac{\overbrace{h_j h_k}^{da}}{h_i}}_{d\ell} \frac{\partial}{\partial q^i} \qquad i,j,k \text{ cyclic} \qquad h_1 h_2 h_3 = \text{Jacobian (weight)}$$

- The Laplacian is manifestly self-adjoint (Hermitian)!
- This gives us a Sturm-Liouville system for each co-ordinate
- Laplacian & free particle solutions: $\mathcal{H}\Psi = E\Psi$ or $(\nabla^2 + k^2)\Psi = 0$ where $E = \frac{\hbar^2 k^2}{2m}$

$$\nabla^2_{cart} = \underbrace{\partial_x^2}_{-k_x^2} + \underbrace{\partial_y^2}_{-k_y^2} + \underbrace{\partial_z^2}_{-k_z^2} \qquad \Psi = e^{i\vec{k}\cdot\vec{r}} = e^{ik_x x} e^{ik_y y} e^{ik_z z} \qquad k^2 = k_x^2 + k_y^2 + k_z^2$$

$$\nabla^2_{cyl} = \underbrace{\frac{1}{\rho}\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho} + \frac{1}{\rho^2}\underbrace{\frac{\partial^2}{\partial\phi^2}}_{-m^2}}_{-k_\rho^2} + \underbrace{\partial_z^2}_{-k_z^2} \qquad \Psi = J_m(k_\rho \rho) e^{im\phi} e^{ik_z z} \qquad k^2 = k_\rho^2 + k_z^2$$

$$\nabla^2_{sph} = \underbrace{\frac{1}{r^2}\frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} + \frac{1}{r^2}\underbrace{\left[\frac{1}{s_\theta}\frac{\partial}{\partial\theta} s_\theta \frac{\partial}{\partial\theta} + \frac{1}{s_\theta^2}\underbrace{\frac{\partial^2}{\partial\phi^2}}_{-m^2}\right]}_{-\ell(\ell+1)}}_{-k_r^2} \qquad \Psi = j_\ell(k_r r) \underbrace{P_\ell^{|m|}(c_\theta) e^{im\phi}}_{\sim Y_{\ell m}(\theta,\phi)} \qquad k^2 = k_r^2$$

* The following operators/eigenvalues are used to reduce these equations: Each of these is a Sturm-Liouville system with eigenvalues & quantization.

+ circular functions: linear (x,y,z) and azimuthal (ϕ) waves:

$$\partial_x e^{ikx} = ik\, e^{ikx} \quad \text{(1st order!)} \qquad \text{or} \qquad -\partial_x^2 \sin(kx) = k^2 \sin(kx) \qquad \int_0^b dx \sin(k_n x)\cdot\sin(k_m x) = \frac{b}{2}\delta_{mn}$$

$$\partial_\phi e^{im\phi} = im\, e^{im\phi} \qquad \text{or} \qquad -\partial_\phi^2 e^{im\phi} = m^2 e^{im\phi} \qquad \int_0^{2\pi} d\phi\, e^{im\phi} e^{im'\phi} = 2\pi\, \delta_{mm'}$$

+ associated Legendre functions: polar (θ) waves (N to S pole)

$$\left[\frac{-1}{s_\theta}\frac{\partial}{\partial\theta} s_\theta \frac{\partial}{\partial\theta} + \frac{m^2}{s_\theta^2}\right] P_\ell^{|m|}(\cos\theta) = \ell(\ell+1)\, P_\ell^{|m|}(\cos\theta) \qquad \int_0^\pi \sin\theta\, d\theta\, P_\ell^{|m|}(x)\, P_{\ell'}^{|m|}(x)$$

$$\text{or } \left[\frac{-\partial}{\partial x}(1-x^2)\frac{\partial}{\partial x} + \frac{m^2}{1-x^2}\right] P_\ell^{|m|}(x) = \ell(\ell+1)\, P_\ell^{|m|}(x) \qquad = \int_{-1}^{1} dx\, P_\ell^{|m|}(x)\, P_{\ell'}^{|m|}(x) = \frac{2\delta_{\ell\ell'}}{2\ell+1}\frac{(\ell+|m|)!}{(\ell-|m|)!}$$

+ Bessel functions: 2-d radial (ρ) waves $\qquad k_n \cdot b = \beta_{mn}$, the n^{th} zero of $J_m(x)$

$$\left[\frac{-1}{\rho}\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho} + \frac{m^2}{\rho^2}\right] J_m(k_\rho \rho) = k_\rho^2 \cdot J_m(k_\rho \rho) \qquad \int_0^b \rho\, d\rho\, J_m(k_n\rho)\cdot J_m(k_{n'}\rho) = \frac{b^2}{2}\delta_{nn'} J_m'^2(\beta_{nm})$$

+ Spherical Bessel functions: 3-d radial (r) waves $\quad k_n \cdot b = \beta_{n\ell}$, n^{th} zero of $j_\ell(x)$

$$\left[\frac{-1}{r^2}\frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} + \frac{\ell(\ell+1)}{r^2}\right] j_\ell(k_r r) = k_r^2\, j_\ell(k_r r) \qquad \int_0^b r^2 dr\, j_\ell(k_n r)\, j_\ell(k_{n'} r) = \frac{b^2}{2}\delta_{nn'}\, j_{\ell\pm1}^2(\beta_{n\ell})$$

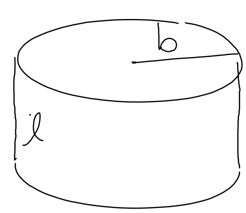
There are other radial functions, one set for each potential $V(r)$, but the angular functions are always the same [rotational symmetry].

* summary of Sturm-Liouville systems: Hermitian operators & orthogonal functions:

$$L|n\rangle = |n\rangle\lambda \qquad \frac{1}{w}\left[\frac{d}{dx}p\frac{d}{dx} - q\right] f_n(x) = \lambda f_n(x) \qquad \langle n|n'\rangle = \int_a^b w\,dx\, f_n^*(x)\, f_{n'}(x) = \delta_{nn'} h_n$$

	$f_n(x)$	index	$a \quad b$	$w\,dx$	$+p$ / $-p$	$+q$ / $-q$	$-\lambda$ / λ	h_n	wave type
i)	$e^{im\phi}$	$m \in \mathbb{Z}$	$0<\phi<2\pi$	$d\phi$	1	0	m^2	2π	(cyl. harmonics)
ii)	$P_\ell^{\lvert m\rvert}(x)$	$\ell=0,1,2\ldots$	$-1<x<1$	dx	$1-x^2$	$\frac{m^2}{1-x^2}$	$\ell(\ell+1)$	$\frac{2}{2\ell+1}\frac{(\ell+\lvert m\rvert)!}{(\ell-\lvert m\rvert)!}$	(sph. harmonics,
	(c_θ)	"	$0<\theta<\pi$	$s_\theta\, d\theta$	s_θ	m^2/s_θ	"	"	polar coords)
iii)	$\sin(k_n x)$	$k_n = \frac{n\pi}{b}$	$0<x<b$	dx	1	0	k_n^2	$\frac{b}{2}$	(linear wave)
iv)	$J_m(k_n\rho)$	$k_n = \frac{\beta_{nm}}{b}$	$0<\rho<b$	$\rho\, d\rho$	ρ	$\frac{m^2}{\rho}$	k_n^2	$\frac{b^2}{2} J_{m\pm1}^2(\beta_{nm})$	(circular wave)
v)	$j_\ell(k_n r)$	$k_n = \frac{\beta_{n\ell}}{b}$	$0<r<b$	$r^2 dr$	r^2	$\frac{\ell(\ell+1)}{r^2}$	k_n^2	$\frac{b^2}{2} j_{\ell\pm1}^2(\beta_{n\ell})$	(spherical wave)
vi)	$Ai(x+x_n)$	$n=1,2,3\ldots$	$0<x<\infty$	dx	1	x	x_0	$Ai'(x_n)^2$	(linear potential)
vii)	$H_n(x)$	$n=0,1,2\ldots$	$-\infty<x<\infty$	$e^{-x^2}dx$	e^{-x^2}	0	$2n$	$\sqrt{\pi}\,2^n n!$	(1-d oscillator)
viii)	$L_n^{(\alpha)}(x)$	$n=0,1,2\ldots$	$0<x<\infty$	$x^\alpha e^{-x}dx$	$x^{\alpha+1}e^{-x}$	0	n	$\frac{\Gamma(\alpha+1+n)}{n!}$	(Harmonic osc. Coulomb potential)

* Example: Free particle confined to a cylinder



$$\frac{-\hbar^2}{2m}\left(\frac{1}{\rho}\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho} + \frac{1}{\rho^2}\frac{\partial^2}{\partial\phi^2} + \frac{\partial^2}{\partial z^2}\right)\psi = E\psi$$

let $\psi(\rho,\phi,z) = J_m(k_\rho \rho)\, e^{im\phi} \sin(k_z z)$ and $E = \frac{\hbar^2 k^2}{2m}$, where $k^2 = k_\rho^2 + k_z^2$

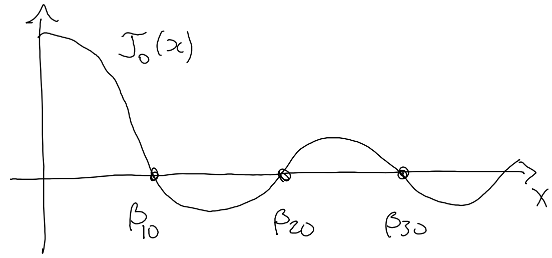
z: $\frac{\partial^2}{\partial z^2} \sin(k_z z) = -k_z^2 \sin(k_z z)$ $\qquad \psi(\rho,\phi,0) = \psi(\rho,\phi,l) = 0$

$\sin(k_z \cdot 0) = 0 \qquad \sin(k_z l) = 0 \Rightarrow k_z l = j\pi, \quad j = 1, 2, 3, \dots$

ϕ: $\frac{\partial^2}{\partial \phi^2} e^{im\phi} = -m^2 e^{im\phi} \qquad \psi(\rho,0,z) = \psi(\rho,2\pi,z) \qquad e^{im0} = e^{im\cdot 2\pi} \Rightarrow m \in \mathbb{Z}$

ρ: $\left(\frac{\partial^2}{\partial \rho^2} + \frac{1}{\rho}\frac{\partial}{\partial \rho} - \frac{m^2}{\rho^2} + k_\rho^2\right) J_m(k_\rho \rho)$ $\qquad$ let $x = k_\rho \rho$

$$\left(\frac{d^2}{dx^2} + \frac{1}{x}\frac{d}{dx} - \frac{m^2}{x^2} + 1\right) J_m(x) = 0$$



This is Bessel's equation, general solution: $A J_m(x) + B Y_m(x)$

$Y_m(x)$ blows up at $x = 0 \rightarrow B = 0$

$\psi(b,\phi,z) = 0 \qquad J_m(k_{mn} b) = 0 \qquad k_{mn} = \frac{\beta_{nm}}{b} \qquad \beta_{nm} = n^{th}$ zero of $J_m(x)$

Thus $\psi_{nmj}(\rho,\phi,z) = N J_m(k_{mn}\rho)\, e^{im\phi} \sin(k_j z) \qquad E_{nmj} = \frac{\hbar^2 k^2}{2m} \qquad k^2 = k_{mn}^2 + k_j^2$

$$\langle n'm'j' | nmj \rangle = |N|^2 \int_0^b \rho\, d\rho\, J_{m'}(k_{n'm'}\rho) J_m(k_{nm}\rho) \int_0^{2\pi} d\phi\, e^{-im'\phi} e^{im\phi} \int_0^l dz \sin(k_{j'} z) \sin(k_j z)$$

$$= |N|^2 \cdot \delta_{n'n} \frac{b^2}{2} J_{m+1}(\beta_{nm}) \cdot \delta_{m'm}\, 2\pi \cdot \delta_{j'j} \frac{l}{2} \quad \Rightarrow \quad N = \sqrt{\frac{2}{\pi b^2 l J_{m+1}(\beta_{nm})}}$$

$$\Psi(\vec{r},t) = \sum_{nmj} c_{nmj}\, \psi_{nmj}(\rho,\phi,z)\, e^{-i\omega t} \quad \text{where } c_{nmj} = \langle nmj | \Psi(\vec{r},0) \rangle$$