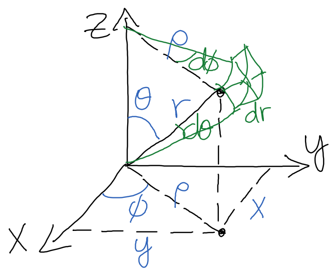
L34-Curvilinear Laplacian Eigenfunctions

Wednesday, December 2, 2015 09:48

* Curvilinear coordinates

$$\begin{array}{ccccc} \text{cart} & & \text{cyl} & & \text{sph} \\ x & = & \rho c_\phi & = & r s_\theta c_\phi \\ y & = & \rho s_\phi & = & r s_\theta s_\phi \\ z & = & z & = & r c_\theta \\ & & \rho & = & r s_\theta \end{array}$$



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

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

- 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 $E = \frac{\hbar^2 k^2}{2m}$

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

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

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

* 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:

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

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

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

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

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

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

$$\left[\frac{-1}{\rho}\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho} + \frac{m^2}{\rho^2}\right] J_m(k\rho) = k^2\, J_m(k\rho) \qquad \int_0^b \ldots J_m(\ldots)\, J_m(\ldots) \ldots \frac{b^2}{2}\delta \ldots J_m'^2(\ldots)$$

+ Bessel functions: 2-d radial (ρ) waves $\quad k_n \cdot b = \beta_{nm}$, 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 $j_\ell(x)$

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

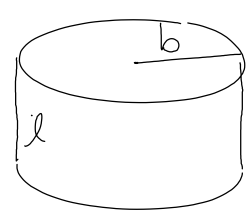
There are other radial functions, one set for each potential $V(r)$, but the angular functions are always the same [rotational symmetry].

* 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 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)	$P_\ell^{\lvert m\rvert}(x)$ (c_θ)	$\ell = 0,1,2\ldots$ "	$-1<x<1$ $0<\theta<\pi$	dx $s_\theta d\theta$	$1-x^2$ s_θ	$\frac{m^2}{1-x^2}$ m^2/s_θ	$\ell(\ell+1)$ "	$\frac{2}{2\ell+1}\frac{(\ell+\lvert m\rvert)!}{(\ell-\lvert m\rvert)!}$ "	(sph. harmonics, polar co-ords)
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	$\frac{b^2}{2}j_{\ell+1}^2(\beta_{n\ell})$	(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



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

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

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 $k^2 = k_\rho^2 + k_z^2$

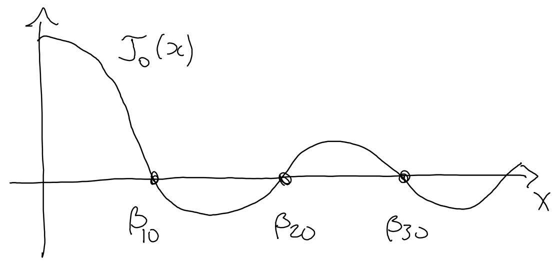
z: $\frac{\partial^2}{\partial z^2}\sin(k_z z) = -k_z^2\sin(k_z z)$ $\qquad \Psi(\rho,\phi,0) = \Psi(\rho,\phi,l) = 0$

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

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: $AJ_m(x) + BY_m(x)$

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

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

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

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