CSF-1

QM Hydrogen atom
$\psi(r,\theta,\phi) = \sum R_n(r) Y_{\ell m}(\theta,\phi)$
ANY WF — Laguerre — Spherical harmonics

Complete sets of functions

You probably have seen Fourier series

ANY periodic function $f(x+2L) = f(x)$

$$f(x) = a_0/2 + \sum_{n=1}^{\infty}\left(a_n \cos\frac{n\pi x}{L} + b_n \sin\frac{n\pi x}{L}\right)$$

$$a_n = \frac{1}{L}\int_0^{2L} \cos\frac{n\pi x}{L} f(x)\,dx$$

$$b_n = \frac{1}{L}\int_0^{2L} \sin\frac{n\pi x}{L} f(x)\,dx$$

Sort of remarkable $\sin\frac{n\pi x}{L}$ and $\cos\frac{n\pi x}{L}$ are a basis for $\boxed{\text{any}}$ periodic function.

We will use this to solve Laplace eqn, but also use $\boxed{\text{OTHER}}$ complete sets of functions.

This suggests it would be nice to have "bigger picture" of where such sets of functions come from!

One place we know complete sets of $\boxed{\text{vectors}}$ arise: eigenvectors of Hermitian matrix.

Is it possible functions $\leftrightarrow$ vectors ?!
What is Hermitian in context of functions ?!

CS# -2

vector $\vec{v}$ components basis $(\hat{e}_1, \hat{e}_2, \hat{e}_3)$

$\begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix}$ ← depend on basis

$\vec{v} = v_1\hat{e}_1 + v_2\hat{e}_2 + v_3\hat{e}_3$

$$\left.\begin{array}{l} \vec{v}+\vec{w} = \vec{w}+\vec{v} \\ \alpha\vec{v} \\ \vec{v}\cdot\vec{v} = \sum v_i^2 \equiv |\vec{v}|^2 \\ \vec{v}+\vec{0} = \vec{v} \\ \vec{v}+(-\vec{v}) = \vec{0} \end{array}\right\}$$ defining properties of vectors

not necessary for vector space but true for ours and most of physics! → $\vec{v}\cdot\vec{v}$

$\boxed{\text{Operator}}$ M takes one vector into another $M\vec{v} = \vec{w}$

Matrix M is array of #'s telling you $\begin{pmatrix} M_{11} & M_{12} & M_{13} \\ M_{21} & M_{22} & M_{23} \\ M_{31} & M_{32} & M_{33} \end{pmatrix}\begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix} = \begin{pmatrix} w_1 \\ w_2 \\ w_3 \end{pmatrix}$

Like components, Depends on basis

Hermition matrix $M_{ij} = M_{ji}^*$ $\Longleftrightarrow$ $v^\dagger M w = (w M v)^*$

More simple real symmetric $M_{ij} = M_{ji}$

Consider $\vec{v} = \hat{e}_i$, $\vec{w} = \hat{e}_j$ to prove $\Longleftarrow$

Eigenvectors of M form a basis

CSF-2A

$$\begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix}\begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = \lambda \begin{pmatrix} v_1 \\ v_2 \end{pmatrix}$$

$$\begin{vmatrix} 2-\lambda & 1 \\ 1 & 2-\lambda \end{vmatrix} = (2-\lambda)^2 - 1 = 0$$

$\lambda = 3 \quad \lambda = 1$

$\lambda = 3 : \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} \equiv \hat{f}_1 \qquad \lambda = 1 : \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix} \equiv \hat{f}_2$

$$\underbrace{\begin{pmatrix} v_1 \\ v_2 \end{pmatrix}}_{\text{components in basis } \begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix}} = \underbrace{\left(\frac{v_1+v_2}{\sqrt{2}}\right)}_{\text{components in eigenbasis}} \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} + \underbrace{\left(\frac{v_1-v_2}{\sqrt{2}}\right)}_{\text{components in eigenbasis}} \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

Notice $\hat{f}_1 \cdot \hat{f}_2 = \phi$ ← another property of real symmetric matrices

NOT SYMMETRIC EXAMPLE:

$$\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}\begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = \lambda \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} \qquad \begin{vmatrix} -\lambda & 1 \\ 0 & -\lambda \end{vmatrix} = \lambda^2 = 0$$

$\Rightarrow \lambda = 0$

$\lambda = 0 \quad \hat{f}_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ ← only eigenvector, not a basis!

CSF-3

$\{$ Continuous functions f on $(0, L)$ $\}$

$f(0) = 0 = f(L)$

Satisfy all defining rules of vectors,

DOT PRODUCT $\quad f \cdot g = \int_0^L f(x)\, g(x)\, dx$

Operator, eg differentiation $\quad \frac{df}{dx} = h$ ← a new continuous function

BASIS $\quad \{1, x, x^2, x^3, \ldots \}$ ← ∞ dimensional

$e^x = 1 + x + \frac{1}{2}x^2 + \frac{1}{6}x^3 + \ldots$

components of e^x in this basis : $\begin{pmatrix} 1 \\ 1 \\ 1/2 \\ 1/6 \\ \vdots \end{pmatrix}$ "=" e^x !!

Other bases? Are there Hermitian operators around?

?! what does this mean

$$\int_0^L f(x)\, \hat{O}\, g(x)\, dx = \int_0^L g(x)\, \hat{O}\, f(x)\, dx$$

Analog of "usual" → $\quad w M v \quad = \quad v M w$

CSF 4

Is $\frac{d}{dx}$ Hermitian?

Try $f(x) = x \quad g(x) = x^2 \quad L = 1$

$$\int_0^1 x \frac{d}{dx} x^2 \, dx \qquad \int_0^1 x^2 \frac{d}{dx} x \, dx$$

$$\int_0^1 2x^2 \, dx \qquad \int_0^1 x^2 \, dx$$

$$\frac{2x^3}{3}\Big|_0^1 \qquad x^3/3 \Big|_0^1$$

$$2/3 \qquad 1/3$$

No!

Eigenfunctions of $\quad d/dx \; e^{\lambda x} = \lambda e^{\lambda x}$

$$\hat{O} f = \lambda f$$

$\{e^{\lambda x}\}$ $\quad$ <u>not</u> <u>a</u> <u>basis</u>

& different λ

CSF-5

how about $\partial^2/\partial x^2$

$$\int_0^{2L} f(x) \frac{d^2}{dx^2} g(x)\, dx$$

integrate by parts

$$= f(x) \frac{d}{dx} g(x) \Big|_0^{2L} - \int_0^{2L} \frac{df}{dx} \frac{dg}{dx}\, dx$$

vanishes if f and g periodic on [0, 2L]

since values at $x = 0, 2L$ identical

$$= -\left(\frac{df}{dx} g \Big|_0^{2L} - \int_0^{2L} \frac{d^2 f}{dx^2} g\, dx \right)$$

$$= \int_0^{2L} g \frac{d^2 f}{dx^2}\, dx$$

$$f \hat{O} g = g \hat{O} f \quad \equiv \text{Hermitian}$$

Example: 5A, B

eigen vectors of $\frac{d^2}{dx^2}$? $\sin kx$, $\cos kx$

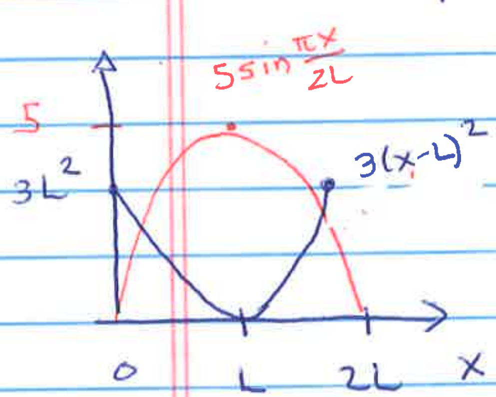
$$d^2/dx^2 \sin kx = -k^2 \sin kx$$

eigenvalue λ

But $k = \frac{\pi n}{L}$ to obey periodicity

CSF-5A

Example: Need $f(x)$ $g(x)$ obeying



$$\left.\begin{array}{l} f(0) = f(2L) \\ g(0) = g(2L) \end{array}\right\} \quad \begin{array}{l} f(x) = 3(x-L)^2 \\ g(x) = 5\sin\frac{\pi}{2L}x \end{array}$$

$$\frac{df}{dx} = 6(x-L) \qquad \frac{d^2f}{dx^2} = 6$$

$$\int_0^{2L} g\frac{d^2}{dx^2}f\,dx = \int_0^{2L} 5\sin\frac{\pi x}{2L}\,6\,dx$$

$$= 30\frac{2L}{\pi}\left(-\cos\frac{\pi x}{2L}\right)\Bigg|_0^{2L} = \frac{60L}{\pi}2 = \frac{120L}{\pi}$$

$$\int_0^{2L} f\frac{d^2}{dx^2}g\,dx = \int_0^{2L} 3(x-L)^2\left(-5\left(\frac{\pi}{2L}\right)^2\sin\frac{\pi x}{2L}\right)dx$$

$$= -\frac{15\pi^2}{4L^2}\int_0^{2L}(x-L)^2\sin\frac{\pi x}{2L}\,dx$$

$u = x - L$

$$-\int_{-L}^{L} u^2\cos\frac{\pi u}{2L}\,du$$

$$\sin\frac{\pi x}{2L} = \sin\left(\frac{\pi u}{2L} - \frac{\pi}{2}\right)$$

$$= -\cos\frac{\pi u}{2L}$$

$$-\int_{-\pi/2}^{\pi/2}\left(\frac{2L}{\pi}\right)^2\theta^2\cos\theta\,\frac{2L}{\pi}\,d\theta$$

$$\theta = \frac{\pi u}{2L}$$

$$= \underbrace{\frac{15\pi^2}{4L^2}\,\frac{8L^3}{\pi^3}}_{\frac{30L}{\pi}}\int_{-\pi/2}^{\pi/2}\theta^2\cos\theta\,d\theta$$

CSF-6

This is the deep theory behind fourier transform

$$\left\{ \sin\frac{n\pi x}{L},\ \cos\frac{n\pi x}{L} \right\}$$ are eigenfunctions of Hermitian operator d^2/dx^2 and are therefore a complete basis

In fact they are even orthogonal!

$$\int_0^{2L} \sin\frac{n\pi x}{L}\sin\frac{m\pi x}{L}\,dx = L\,\delta_{nm}$$

This is why

$$b_n = \frac{1}{L}\int_0^{2L} \sin\frac{n\pi x}{L} f(x)\,dx$$

Obvious question: Is d^2/dx^2 unique or are there other Hermitian operators? If answer is yes, then there are other complete sets of functions

Legendre, Hermite, Bessel, ... !!!!
Laguerre, ...

CSF-7

2nd order linear differential operator

$$\mathcal{L} = p_0(x)\frac{d^2}{dx^2} + p_1(x)\frac{d}{dx} + p_2(x)$$

Just say calculation in words!

$$\langle f|\mathcal{L}|g\rangle \equiv \int_a^b dx\, f(p_0 g'' + p_1 g' + p_2 g)$$

$$\langle g|\mathcal{L}|f\rangle \equiv \int_a^b dx\, g(p_0 f'' + p_1 f' + p_2 f)$$ try to match

$$= \int_a^b dx\left[-(g p_0)' f' - (g p_1)' f + p_2 f g\right] + g p_0 f' + g p_1 f \Big|_a^b$$

$$= \int_a^b dx\left[(g p_0)'' f - (g p_1)' f + p_2 f g\right] + g p_0 f' + g p_1 f - (g p_0)' f \Big|_a^b$$

$$(g' p_0 + g p_0')' = g'' p_0 + 2 g' p_0' + g p_0''$$

$$+ g p_0 f' + g p_1 f - (g p_0)' f \Big|_a^b$$

$$\langle g|\mathcal{L}|f\rangle = \int_a^b dx\left[g'' p_0 + 2g' p_0' + g p_0''\right] f - (g' p_1 + g p_1') f + p_2 f g$$

$$\langle f|\mathcal{L}|g\rangle = \int_a^b dx\left[f p_0 g'' \qquad + g' p_1 f \qquad + p_2 f g\right]$$

The difference is

vanishes if $p_1 = p_0'$

$$\langle g|\mathcal{L}|f\rangle - \langle f|\mathcal{L}|g\rangle = \int_a^b dx\left[f(2p_0' - 2p_1)g' + f(p_0'' - p_1')g\right]$$

bdy term $\leadsto$ $g p_0 f' + g p_1 f - (g p_0)' f \Big|_a^b$ if $p_1 = p_0'$

$$g p_0 f' + g p_1 f - g' p_0 f - g p_0' f \Big|_a^b$$

$$p_0 (g f' - g' f)$$

So $\mathcal{L}$ is Hermitian if

(1) $p_1 = p_0'$

(2) $gf' - f'g \Big|_a^b = 0$

possible boundary conditions

Dirichlet : f, g vanish at a, b

Neumann : f', g' " " "

periodic : $f(a) = f(b)$ $f'(a) = f'(b)$ + similarly for g

CSF-8A

Slight complication:

$$\mathcal{L}\, u(x) = \lambda\, w(x)\, u(x)$$

"Generalized Eigenvalue problem"

"weight function"

Hermiticity condition $\quad p_1(x) = \frac{1}{w}\frac{d}{dx}(w p_0)$

Inner product $\quad \langle f|\mathcal{L}|g\rangle \equiv \int_a^b f(x)g(x)w(x)dx$

determines $p_1(x)$

	$p_0(x)$	$p_2(x)$	$w(x)$
Fourier	1	ϕ	1
Legendre	$1-x^2$	0	1
Hermite	e^{-x^2}	ϕ	e^{-x^2}
Bessel	x	$-n^2/x$	x
Laguerre	xe^{-x}	ϕ	e^{-x}
Chebyshev			
Gegenbauer			
⋮			