Lecture 5 Special Functions

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Sturm - Liouville Theory - Orthogonal Expansions

- We have already seen that Fourier series $\{\sin \frac{n\pi x}{L}, \cos \frac{n\pi x}{L}\}$ are useful in the description of physical process in rect. angular coordinates.

  e.g. waves on a string
  particle in a square box.

- They appear so often is because they are eigenfunctions of the ∇^2 operator in rect. coord.

Laplace EM: $\nabla^2 \phi = 0$

Helmholtz QM: $H\psi = E\psi$, $H = -\frac{\hbar^2}{2m}\nabla^2 + V_0$

$$\rightarrow \nabla^2\psi = -\frac{2m}{\hbar^2}(E - V_0)\psi$$

$$\nabla^2\psi = -k^2\psi$$

Rectangular coordinates

$\nabla^2\phi = 0$ Electrostatic problems in Rect.

We usually solve this by seperation of variables

$$\nabla^2\phi = \frac{\partial^2}{\partial x^2}\phi + \frac{\partial^2}{\partial y^2}\phi = 0$$

– Let $\phi(x,y) = X(x)\,Y(y)$

then
$$\nabla^2\phi = Y\frac{d^2}{dx^2}X + X\frac{d^2}{dy^2}Y = 0$$

$$\underbrace{\frac{1}{X}\frac{d^2}{dx^2}X}_{\text{fn of } x \text{ only}} + \underbrace{\frac{1}{Y}\frac{d^2}{dy^2}Y}_{\text{fn of } y \text{ only}} = 0$$

$$\Rightarrow \quad \frac{1}{X}\frac{d^2}{dx^2}X = -\alpha^2 \quad \text{and} \quad \frac{1}{Y}\frac{d^2}{dy^2}Y = \alpha^2$$

☆ This gives sine & cosine as eigenfunctions. (fund. solutions)
sinh cosh

☆ Numerically, tri functions are easy to calculate.
we usually don't talk about them in comp. tech.

- On the other hand, if ∇^2 is in a different coordinates or $V(x) \neq V_0$, then the types of eigenfunctions change!

☆ As stated before, the set of eigenfunctions depends on the operator $H(\nabla^2, V)$ and the domain of interest.

General Form

These discussion is usually put in the form of the eigenfns and eigenvalues of a "self-adjoint" operator.

$$\mathcal{L}\, u(x) + \lambda\, w(x)\, u(x) = 0$$

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

then $\mathcal{L}$ is self adjoint iff $p_0'(x) = p_1(x)$.

Then, $\mathcal{L}$ can be written in the following form:

$$\mathcal{L} u(x) = \frac{d}{dx}\left[p(x) \frac{du(x)}{dx} \right] + q(x)\, u(x).$$

With $p_0(x) \neq 0$ in $[a,b]$, any non-self-adjoint operator can be put into self-adjoint form by multipling $\mathcal{L}$ by (4)

$$\frac{1}{p_0(x)} \exp\left[\int^x \frac{p_1(t)}{p_0(t)}\,dt\right]$$

$$\frac{1}{p_0} \exp\left[\int^x \frac{p_1}{p_0}\,dt\right] \mathcal{L}u(x) = \frac{d}{dx}\left\{\exp\left[\int^x \frac{p_1}{p_0}\,dt\right]\frac{du}{dx}\right\} + \frac{p_2}{p_0}\exp\left[\int^x \frac{p_1}{p_0}\,dt\right]u$$

For most physical system, ODE can be put in the self-adjoint form:

(*) $\mathcal{L}u(x) + \lambda w(x) u(x) = 0$

λ - eigenvalues

$w(x)$ - weighting function

$u_\lambda(x)$ - eigen functions

— λ is an eigenvalue and $u_\lambda(x)$ is a eigenfunction of (*) if they satisfies (*) <u>AND</u> the given B.C. !

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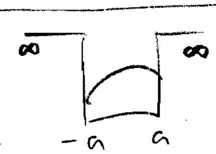
e.g.



$\mathcal{L} = \frac{d^2}{dx^2}$ $\quad w(x) = 1$, $p(x) = 1$, $q(x) = 0$

sin, cos

B.C. $u(\pm a) = 0$

$u'(\pm a) = 0$

☆ However, $u_\lambda(x)$ does not exist for <u>all choices of λs</u>!

<u>Physics Notes</u>:

In fact, the requirement for $u_\lambda(x)$ to exist, there can only be a set of acceptable values for λ!

$\Rightarrow$ Mathematical basis for Quantization!

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examples:	$p(x)$	$q(x)$	λ	$w(x)$
Legendre	$1-x^2$	0	$\ell(\ell+1)$	1
ass Legendre	$1-x^2$	$-\frac{m^2}{1-x^2}$	$\ell(\ell+1)$	1
Bessel	x	$-\frac{\nu^2}{x}$	a^2 (1) if $x=k\ell$	x
Hermite	e^{-x^2}	0	$2\lambda+1$ (odd)	e^{-x^2}
Simple Harmonic (Fourier series)	1	0	n^2	1

Linkage of Self-Adjoint operators to orthogonal functions

Important properties of Hermitian / Self-Adjoint operators:

all QM are discribled by Hermitian Operators

$H = (H^{+})^{*}$

transpose ⊕ complex conjugate

(Hermitian is Self-Adjoint)

① - λ_n's are real numbers

② - $u_n(x)$ are orthogonal

$$\int_a^b u_n(x)\, u_m(x)\, w(x)\, dx = \delta_{nm} C_m$$

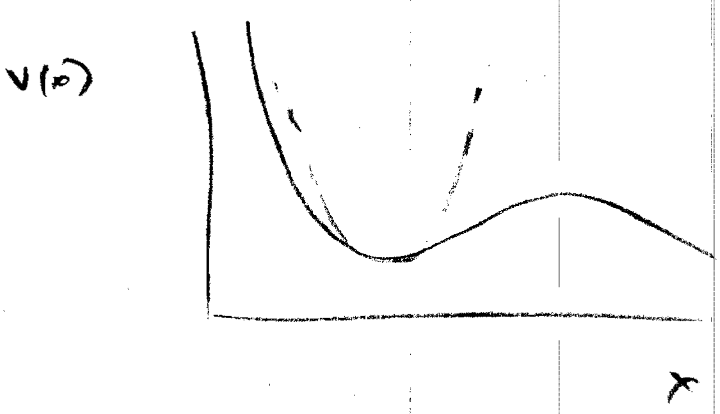
③ - $u_n(x)$ form a complete set

$$f(x) = \sum_m a_m u_m(x)$$

Hermite Polynomial & Harmonic Oscillator

$$V_{ho}(x) = \frac{1}{2} M \omega^2 x^2$$

☆ – This is important because for any $V(x)$ with a minimum, it can be app. locally by $V_{ho}(x)$



1D harmonic oscillator

$$H = \frac{1}{2M} P_x^2 + \frac{1}{2} M \omega^2 x^2$$

$$H \psi(x) = E \psi(x)$$

$$\rightarrow \quad -\frac{\hbar^2}{2M^2} \frac{d^2\psi(x)}{dx^2} + \left(\frac{1}{2} M \omega^2 x^2 - E\right) \psi(x) = 0$$

$E \to \lambda = \frac{E}{\frac{1}{2}\hbar\omega}$ ▸ rescale energy by $\frac{1}{2}\hbar\omega$

$\rho = \sqrt{\frac{m\omega}{\hbar}}\, x$ dimensionless length scale

$$\frac{d^2\psi}{d\rho^2} + (\lambda - \rho^2)\psi(\rho) = 0$$

This is related to the Hermite Diff Eq if we substitute

$\psi(\rho) = A\, e^{-\rho^2/2} H(\rho)$ into the below eq.

$$H''(\rho) - 2\rho H'(\rho) + (\lambda - 1) H(\rho) = 0 \quad (*)$$

← related to $P(x)$, $w(x)$ in table (see note on 7′)

(This can be put into self adjoint form by ⊗ $e^{-\rho^2}$)

~~(*) has eigenvalues λ = odd integers~~

~~$\Rightarrow E_n = (2n+1)\frac{1}{2}\hbar\omega$ (see above)~~

~~$H_n(\rho) = \sum_{k=0,1\ (\text{even/odd})}^{n} a_{n,k}\rho^k$, $a_{n,k+2} = \frac{2k-\lambda+1}{(k+1)(k+2)} a_{n,k}$~~ ↑ Note!

✓✓ ~~(either even or odd powers)~~

are the Hermite polynomials.

– From Harmonic oscillator eq to Hermite diff Eq.

$$H''(\rho) - 2\rho H'(\rho) + (\lambda-1)H(\rho) = 0 \qquad (*)$$

let $H(\rho)\, e^{-\rho^2/2} = \psi(\rho)$

$$H(\rho) = e^{\rho^2/2}\psi(\rho)$$

$$H'(\rho) = \rho e^{\rho^2/2}\psi + e^{\rho^2/2}\psi'(\rho)$$

– $H''(\rho) = e^{\rho^2/2}\psi + \underline{\rho^2 e^{\rho^2/2}\psi} + \underline{\rho e^{\rho^2/2}\psi'} + \underline{\rho e^{\rho^2/2}\psi'} + e^{\rho^2/2}\psi''$

– $-2\rho H'(\rho) = \underline{-2\rho^2 e^{\rho^2/2}\psi} - \underline{2\rho e^{\rho^2/2}\psi'(\rho)}$

– $(\lambda-1)H(\rho) = (\lambda-1)e^{\rho^2/2}\psi$

put these into $(*)$:

$$e^{\rho^2/2}\psi'' - \rho^2 e^{\rho^2/2}\psi + e^{\rho^2/2}\lambda\psi = 0$$

$$\Rightarrow \qquad \psi'' + (\lambda-\rho^2)\psi = 0 \qquad \leftarrow \text{Harmonic oscillator Eq}$$

– To put Hermite Diff. Eq into Self-Adjoint form :

$(\times)\ e^{-\rho^2}$ to $(*)$:

$$e^{-\rho^2}H'' - 2\rho e^{-\rho^2}H' + e^{-\rho^2}(\lambda-1)H = 0$$

$$\underbrace{\left[e^{-\rho^2}\frac{d^2}{d\rho^2} - 2\rho e^{-\rho^2}\frac{d}{d\rho} - e^{-\rho^2}\right]}_{(\text{self-adj})\ \mathcal{L}} H + e^{-\rho^2}\lambda H = 0 \qquad \left[\frac{d}{d\rho}\left(e^{-\rho^2}\right) = -2\rho e^{-\rho^2}\right]$$

$$\mathcal{L}H + w(\rho)\lambda H = 0$$

- Soln to the Hermite Diff. Eq:

- Assume a series soln to $H(\rho) = \sum_{k=0}^{\infty} a_k \rho^k$

put this into ⊛ & equating coefficients with like powers :

see next page

$$a_{k+2} = \frac{2k+1-\lambda}{(k+1)(k+2)} a_k$$

- Since we want the series to remain finite for arbitrary ρ, need the series must terminate after a finite # of terms!

$$\Rightarrow \quad \lambda = 2n+1 \qquad \text{where } n \in \mathbb{Z}$$

→ ⊛ has eigenvalues : λ_n = odd integers

$$E_n = (2n+1)\frac{1}{2}\hbar\omega \qquad (\lambda = E/\tfrac{1}{2}\hbar\omega)$$

⊛ has eigenfunctions : $H_n(\rho) = \sum_{k=0}^{n} a_{n,k}\rho^k$ (Hermite polynomials)

where $a_{n,k+2} = \dfrac{2k+1-\lambda_n}{(k+1)(k+2)} a_{n,k}$

Note: Hermite polynomials exist for all n and for n even, the series soln will start with $a_{n,0} \neq 0$, $a_{n,1} = 0$

n odd, $a_{n,0} = 0$, $a_{n,1} \neq 0$

(actual coefficients are fixed by normalization).

Series soln to $H_n(\rho)$:

let $H(\rho) = \sum_{k=0}^{\infty} a_k \rho^k$

$$\begin{cases} H'(\rho) = \sum_{k=0}^{\infty} k a_k \rho^{k-1} \\ H''(\rho) = \sum_{k=0}^{\infty} k(k-1) a_k \rho^{k-2} \end{cases}$$

- Substitute these into $\circledast$:

$$\sum_{k=0}^{\infty} k(k-1) a_k \rho^{k-2} - 2\rho \sum_{k=0}^{\infty} k a_k \rho^{k-1} + (\lambda - 1) \sum_{k=0}^{\infty} a_k \rho^k = 0$$

$\Downarrow$ $\nexists$ ρ^{-2} & ρ^{-1} terms $\qquad$ $\Downarrow$ multiply ρ into sum

$$\sum_{k=2}^{\infty} k(k-1) a_k \rho^{k-2} \qquad - 2 \sum_{k=0}^{\infty} k a_k \rho^k$$

- shifting index to compare terms with like powers of ρ:

$$\sum_{k=0}^{\infty} (k+2)(k+1) a_{k+2} \rho^k - \sum_{k=0}^{\infty} (2k - \lambda + 1) a_k \rho^k = 0$$

- For this to be valid for all terms with like powers:

$$(k+2)(k+1) a_{k+2} = (2k - \lambda + 1) a_k$$

$$a_{k+2} = \frac{2k - \lambda + 1}{(k+2)(k+1)} a_k$$

~~Note: With $\lambda = 2n+1$ the series terminates at $k=n$! for a given n.~~

— Just like the <u>sins</u> & <u>cosines</u>:

$\exists$ are two linear independent sets of solns.

$\sim$ k even or k odd.

$a_0 \neq 0 \quad a_1 = 0$ $\qquad$ $a_1 \neq 0 \quad a_0 = 0$

Orthogonality condition:

$$\int_{-\infty}^{\infty} e^{-\rho^2} H_n(\rho) H_m(\rho)\, d\rho = 2^n n! \sqrt{\pi}\, \delta_{n,m}.$$

Completeness:

$H_n(\rho)$ forms a complete set

$$\rightarrow \quad f(\rho) = \sum_{k=0}^{\infty} C_k H_k(\rho)$$

Recursion relation: A method to generate H_n:

$(\lambda = 2n+1 \Rightarrow (\lambda - 1) = 2n)$

$$H_{n+1}(\rho) = 2\rho H_n(\rho) - 2n H_{n-1}(\rho)$$

with $H_0 = 1$; $H_1 = 2\rho$

or

$$\Rightarrow \quad a_{n+1,k} = 2a_{n,k-1} - 2n\, a_{n-1,k}$$

$\leftarrow$ Equating terms with like powers of ρ.

Thus, with H_n & H_{n-1}, we can get H_{n+1}!

example: $H_0(\rho) = 1$

$H_1(\rho) = 2\rho$

$a_{0,0} = 1$

$a_{1,0} = 0$

$a_{1,1} = 2$

$$\Rightarrow \quad a_{2,0} = 2\cancel{a_{1,-1}}^{\,0} - 2n\, a_{0,0} = -2$$

$$a_{2,1} = 2a_{1,0} - 2\cancel{a_{0,1}}^{\,0} = 0$$

$a_{n,k} = 0$ for $k > n$

$$a_{2,2} = 2a_{1,1} - 2\cancel{a_{0,2}}^{\,0} = 4$$

$$\Rightarrow \quad H_2(\rho) = 4\rho^2 - 2$$

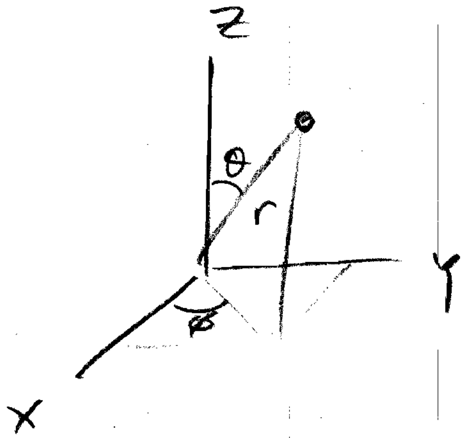
Alternative Way: — use Numerical values of H_n itself.

$$H_2(\rho) = 2\rho H_1(\rho) - 2H_0(\rho)$$

★ Typically, for large value of n, the method with coefficients is more robust!

Legendre Polynomials & Spherical Harmonics

Problems with sphereical symmetry



$\nabla^2 \Phi = 0$ Laplace

$(\nabla^2 + k^2)\psi = 0$ Helmholtz

in spherical coordinates.

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]$$

In Q M, $\quad \frac{1}{\hbar^2}L^2 = -\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]$

(angular momentum operator)

Again, by seperation of variable we have

$$\psi(r) = \frac{R(r)}{r}Y(\theta,\phi)$$

$$\nabla^2\left(\frac{R(r)}{r}Y(\theta,\phi)\right)$$

$$\downarrow$$

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)\left(\frac{R}{r}Y\right) = Y\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\overbrace{\left(\frac{1}{r}\frac{\partial R}{\partial r}-\frac{R}{r^2}\right)}^{\frac{\partial}{\partial r}\left(\frac{R}{r}\right)}\right)\right]$$

$$= Y\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r\frac{\partial R}{\partial r}-R\right)\right]$$

$$= Y\left[\frac{1}{r^2}\left(\cancel{\frac{\partial R}{\partial r}}+r\frac{\partial^2 R}{\partial r^2}-\cancel{\frac{\partial R}{\partial r}}\right)\right]$$

$$= Y\left(\frac{1}{r}\frac{\partial^2 R}{\partial r^2}\right)$$

$$\frac{1}{r^2}[\quad]\left(\frac{R}{r}Y\right) = \frac{R}{r^3}[\quad]Y$$

$$\frac{r^3}{RY}\left[Y\left(\frac{1}{r}\frac{\partial^2 R}{\partial r^2}\right)+\frac{R}{r^3}[\ ]Y\right] = 0$$

$$\underbrace{\frac{r^2}{R}\frac{\partial^2 R}{\partial r^2}}_{\ell(\ell+1)} + \underbrace{\frac{1}{Y}[\ ]Y}_{-\ell(\ell+1)} = 0$$

~~Case 1~~: $\nabla^2 \varphi = 0$

$$\frac{d^2 R}{dr^2} - \frac{\ell(\ell+1)}{r^2} R = 0 \qquad \text{radial} \qquad \left(R \sim \begin{cases} r^{-\ell} \\ r^{\ell+1} \end{cases} \right)$$

$$\left[\frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \left(\sin\theta \frac{\partial}{\partial\theta} \right) + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2} \right] Y(\theta,\phi) = -\ell(\ell+1) Y(\theta,\phi)$$

angular

Case 2: $\nabla^2 \psi + k^2 \psi = 0$

$$\cancel{\frac{d}{dr}\left(r^2 \frac{d}{dr}\right) R(r) + (kr)^2 R(r) = \ell(\ell+1) R} \qquad \text{radial}$$

same angular part as before.

→ In this case, we are interested in the angular part for both cases :

$Y(\theta,\phi)$ can be further separated

$$Y(\theta,\phi) = P(\theta)\,\Phi(\phi)$$

↑

spherical harmonics (we will get back to them later)

$$\begin{cases} \dfrac{1}{P(\theta)\sin\theta}\dfrac{d}{d\theta}\left(\sin\theta\dfrac{d}{d\theta}\right)P(\theta) + \ell(\ell+1) - \dfrac{m^2}{\sin^2\theta} = 0 \quad (*) \\ \dfrac{1}{\Phi(\phi)}\dfrac{d^2}{d\phi^2}\Phi(\phi) = -m^2 \end{cases}$$

The second one is simple & we have seen it before, the eigenfunction for $\Phi(\phi)$ are $e^{im\phi}$, $e^{-im\phi}$.

$$\Rightarrow \Phi(\phi) = Ae^{im\phi} + Be^{-im\phi} \quad (\text{or sines or cosines})$$

☆ since ϕ is a angular variable in $[0, 2\pi]$, and $\Phi(\phi)$ is periodic in $[0, 2\pi]$:

$\Rightarrow$ m must be integers

Legendre Equations

let $\eta = \cos\theta \rightarrow (*)$, we have

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

$\eta \in [-1, 1]$ $\qquad\qquad$ $\dfrac{d}{d\eta} = -\dfrac{1}{\sin\theta}\dfrac{d}{d\theta}$

$$\frac{1}{P(\theta)}\underset{\substack{\uparrow\\ -\frac{d}{d\eta}}}{\left(\frac{1}{\sin\theta}\frac{d}{d\theta}\right)}\left[\underset{\substack{\uparrow\\ 1-\eta^2}}{\sin^2\theta}\underset{\substack{\uparrow\\ -\frac{d}{d\eta}}}{\left(\frac{1}{\sin\theta}\frac{d}{d\theta}\right)}\right]P(\theta) = -\ell(\ell+1) + \frac{m^2}{\underset{1-\eta^2}{\sin^2\theta}}$$

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

Simplier case, $m=0$ (no ϕ dependence)
Azimutal symmetric

$$\frac{d}{d\eta}\left[(1-\eta^2)\frac{dP}{d\eta}\right] + \ell(\ell+1)P(\eta) = 0$$

(Lengendre Equation)

($m \neq 0$, associated Lengendre Eq.)

The solution are the Lengendre Polynomials
(for ℓ integers)

$$P_\ell(\eta) = \sum_{k=0,1}^{\ell} a_{\ell,k}\,\eta^k$$

$$a_{\ell,k+2} = \frac{k(k+1) - \ell(\ell+1)}{(k+1)(k+2)}\,a_{\ell,k},$$

again, for a particular ℓ, the series terminates at $k=\ell$.

Similar to Hermite, $P_\ell(\eta)$ are of even or odd powers!

Orthogonality condition:

$$\int_{-1}^{1} P_m(\eta)P_n(\eta)\,d\eta = \frac{2}{2n+1}\,\delta_{m,n}.$$

$$P_0(\eta) = 1; \quad P_1(\eta) = \eta$$

Numerical recurrence for Legendre Poly
(stable)

$$\Rightarrow P_{n+1}(x) = 2xP_n(x) - P_{n-1}(x) - [xP_n(x) - P_{n-1}(x)]/(n+1)$$

start with $P_0(x) = 1$

$P_1(x) = x$

[Arfken P. 647]

then iterate upward.

Recursion relations

$$(2k+1)\eta P_k(\eta) = (k+1)P_{k+1}(\eta) + k P_{k-1}(\eta)$$

☆ Be aware that recurrence relations are not necessary stable against round off error in the direction where we want to go (increasing n or decreasing n)

☆ [it is a dynamical equation, a particular "trajectory" $\{P_k\}$ might be exponentially sensitive to perturbation]

i.e. $X_{n+1} = 2 X_n \pmod 1$

starting with $X_0 = 0$ will give you $X_n = 0 \ \forall n$.

but $X_0 = \epsilon$, X_n will be chaotic.