Basis functions : Sturm-Liouville Theory

The Fourier representation is very useful for solving differential equations in rectangular coordinates x, y, z. We need to develop similar techniques for other coordinate systems — spherical and cylindrical.

The Fourier representation is appropriate in a normal rectangular system because e^{ikx} is the eigenfunction of the $\frac{\partial}{\partial x}$ operator, e.g.

$$\frac{\partial}{\partial x}\left(e^{ikx}\right) = ik\left(e^{ikx}\right)$$

To extend this concept to other geometries must develop a procedure for obtaining eigenfunctions in other geometries.

Consider the operator

$$\mathcal{L}\, y = a_2(x)\frac{d^2}{dx^2}y + a_1(x)\frac{dy}{dx} + a_0(x)\,y$$

defined over the interval (a, b) where $a_2(x) \neq 0$ for $a < x < b$ but can have $a_2(a) = 0$ or $a_2(b) = 0$. Take a_0, a_1, a_2 to be real. No singular points interior to (a, b).

Define an adjoint operator

$$\bar{\mathcal{L}} y = \frac{d^2}{dx^2} a_2 y - \frac{d}{dx} a_1 y + a_0 y$$

If the operator is self-adjoint $(\bar{\mathcal{L}} = \mathcal{L})$ we must have

$$\bar{\mathcal{L}} y = a_2 y'' + (2a_2' - a_1) y' + (a_2'' - a_1' + a_0) y$$

$$= a_2 y'' + \quad a_1 \quad y' + a_0 y$$

$$2a_2' - a_1 = a_1 \quad \Rightarrow \quad a_2' = a_1$$

so

$$\mathcal{L} y = a_2 y'' + a_2' y + a_0 y$$

$$= \frac{d}{dx}\left(a_2 \frac{d}{dx} y\right) + a_0 y$$

If the equation is not originally self-adjoint can make it self-adjoint by multiplying by

$$\frac{1}{a_2(x)} e^{\int^x dx' \frac{a_1(x')}{a_2(x')}}$$

Thus, assume that $\mathcal{L}$ is self-adjoint and of the form

$$\mathcal{L}y = \frac{d}{dx} P(x) \frac{d}{dx} y + q(x)\, y$$

with $p > 0$ except possibly at "a" or "b".

Suppose that y satisfies the equation

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

with λ a constant and w the <u>weight</u> function $w(x) > 0$ except possibly at isolated points where $w = 0$. For certain values λ_n, y_n satisfies the required boundary conditions at a, b. y_n is the eigenfunction and λ_n is the eigenvalue.

<u>example</u> Legendre's Equ.

$$(1-x^2)\,y'' - 2x\,y' + \ell(\ell+1)\,y = 0$$

$$\frac{d}{dx}(1-x^2)\frac{dy}{dx} + \ell(\ell+1)\,y = 0$$

For this case $P(x) = 1-x^2$, $q(x) = 0$, $w = 1$ and $\lambda = \ell(\ell+1)$.

Why are self-adjoint operators important? Consider two solutions y and g of the equations

$$\mathcal{L} y + \lambda w y = 0$$
$$\mathcal{L} g + \lambda w g = 0$$

where the eigen values may differ. Consider the integral

$$\int_a^b dx\, g^* \mathcal{L} y = \int_a^b dx\, g^* (p y')' + \int_a^b dx\, q g^* y$$

$$= g^* p y' \Big|_a^b - \int_a^b dx\, p y' g^{*\prime} + \int_a^b dx\, q g^* y$$

Choose B.C.s such that

$$p(x) g^*(x) y'(x) \Big|_a^b = 0$$

$\Rightarrow$ could be satisfied by conditions on g, y or p. Another integration by parts

$$\int_a^b dx\, g^* \mathcal{L} y = -p y g^{*\prime} \Big|_a^b + \int_a^b dx\, y (p g^{*\prime})' + \int_a^b dx\, q g^* y$$

Again take

$$p y g^{*\prime} \Big|_a^b = 0$$

$$\boxed{\int_a^b dx\, g^* \mathcal{L} y = \int_a^b dx\, y \mathcal{L} g^*}$$

This property allows us to generate a set of orthogonal function

Hermitian Operators

More generally the operator $\mathcal{L}$ might be complex. For example in quantum mechanics

$$P_x = -i\hbar \frac{\partial}{\partial x}$$

In this case we define a Hermitian operator as follows

$$\int_a^b dx\, g^* \mathcal{L} y = \int_a^b dx\, y\, (\mathcal{L} g)^*$$

For $\mathcal{L}$ real this is the same as our definition of self-adjoint operators.

The expectation value of an operator $\mathcal{L}$ is given by

$$\langle \mathcal{L} \rangle \equiv \frac{\int_a^b dx\, \psi^* \mathcal{L} \psi}{\int_a^b dx\, \psi^* \psi}$$

where ψ is the wave function of the system. Any observable must be real so

$$\langle \mathcal{L} \rangle^* = \frac{\int_a^b dx\, \psi\, \mathcal{L}^* \psi^*}{\int_a^b dx\, \psi^* \psi}$$

If $\mathcal{L}$ is Hermitean,

$$\langle \mathcal{L} \rangle^* = \frac{\int_a^b dx\, \psi^*(\mathcal{L}\psi)}{\int_a^b dx\, |\psi|^2} = \langle \mathcal{L} \rangle$$

$\Rightarrow$ any operator $\mathcal{L}$ which corresponds to an observable quantity must be Hermitean.

Eigenfunctions from Self-Adjoint Operators

Consider the equation

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

$$\mathcal{L} = \frac{\partial}{\partial x} p \frac{\partial}{\partial x} + g(x)$$

For any value of λ have two solutions

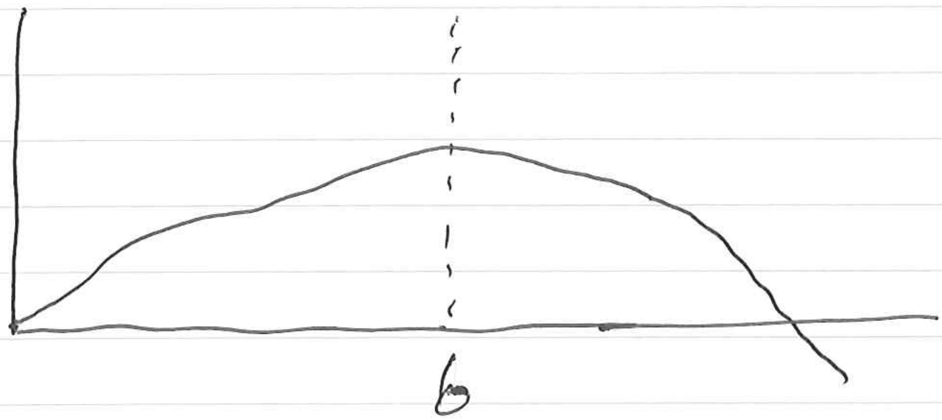
$$y = c_1 \psi_1(x) + c_2 \psi_2(x)$$

Choose one boundary at $x=a$. Can always choose

$$y(a) = 0 = c_1 \psi_1(a) + c_2 \psi_2(a)$$

$\Rightarrow$ assume "a" is not a sing. pt. of the eqn.

Suppose y looks like the following with $p>0$,



We want to vary λ to match the B.C. at $x=b$

$\Rightarrow$ e.g., $y(b)=0$

If we increase λ, the solution becomes more oscillatory

$$\frac{\partial}{\partial x} p \frac{\partial}{\partial x} y + q y + \lambda w y = 0$$

$\Rightarrow$ this is more obvious if we simply take $p=1$, $q=0$ and $w=1$

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

$$y \sim e^{\pm i \lambda^{1/2} x}$$

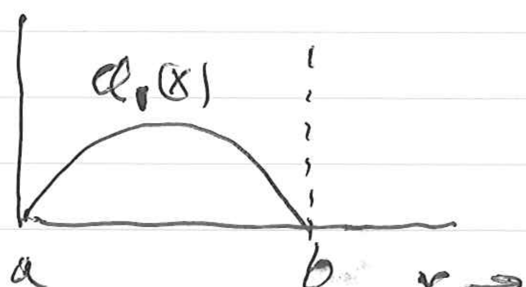
$\Rightarrow$ increasing λ makes the wavevector $k=\lambda^{1/2}$ larger and the wavelength ~~the~~ shorter

$\Rightarrow$ zero point of y moves to the left above.

$\Rightarrow$ a general property of the self-adjoint equation is that increasing λ causes the zero point to shift to the left.

$\Rightarrow$ increase λ until $y(b) = 0$

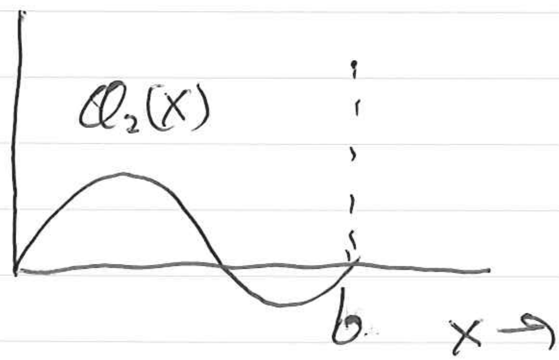
$\Rightarrow$ defines the first eigenvalue λ_1 and eigenfunction $\varphi_1(x)$

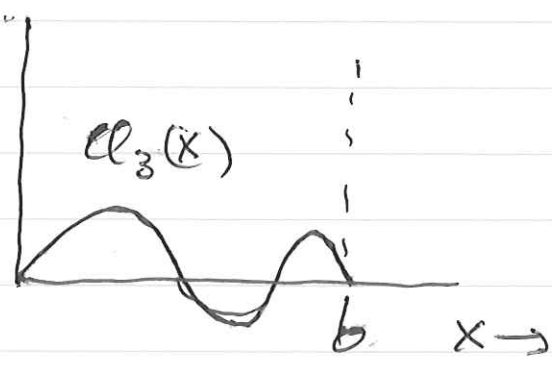


$\Rightarrow$ increase λ further until the second zero of y intersects $x = b$.

$\Rightarrow$ yields $\lambda_2, \varphi_2(x)$

$\Rightarrow$ continue to λ_3, φ_3





example

$$\frac{d^2 y_n}{dx^2} + k_n^2 y_n = 0$$

What are the solutions on (a, b)?

$\Rightarrow$ require $\quad y_n y_m' \Big|_a^b = 0$

Take

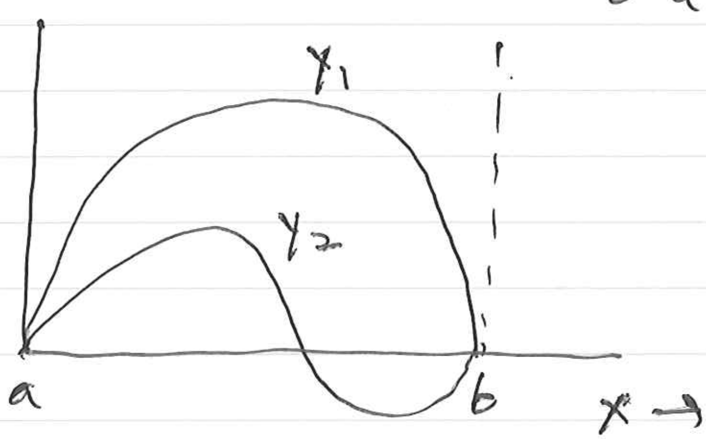
$$y_n(a) = 0, \quad y_n(b) = 0$$

$$y_n(x) = \sin k_n(x-a)$$

$$y_n(b) = 0 = \sin[k_n(b-a)]$$

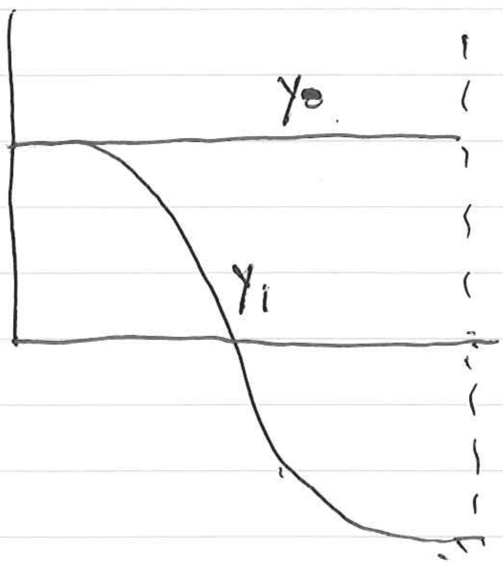
$$k_n = \frac{n\pi}{b-a}$$

$$y_n = \sin\left[\frac{n\pi(x-a)}{b-a}\right]$$



Or can take $y_n'(a) = y_n' b = 0$

$$y_n(x) = \cos\left(\frac{n\pi(x-a)}{b-a}\right)$$

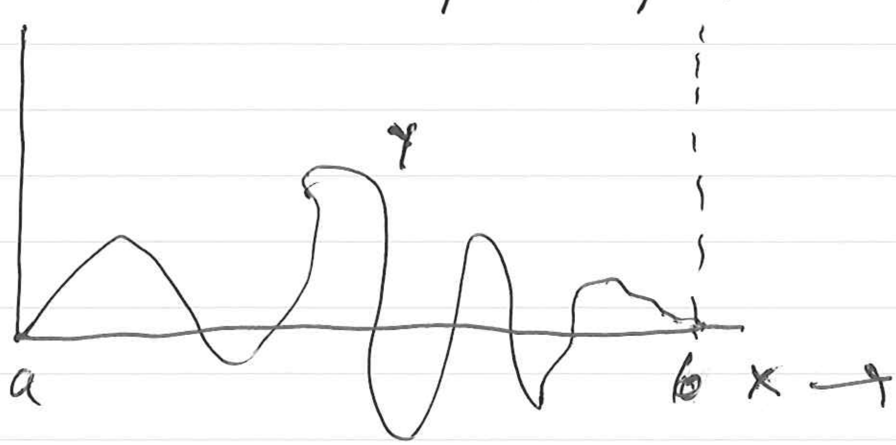


$\Rightarrow$ a separate set of basis functions

$\Rightarrow$ different BCs yield a different sequence of functions

$\Rightarrow$ choose B.Cs to match the problem of interest

$\Rightarrow$ e.g. for vibrating string might want $y(a) = y(b) = 0$



Properties of self-adjoint or Hermitian operators

1) Eigenvalues of Hermitian operators are real

2) Eigenfunctions of a Hermitian operator are orthogonal

$\Longrightarrow$ automatic if B.C.s are satisfied

$$p(x)\, y_n\, y_m'^{*} \Big|_a^b = 0$$

3) Eigenfunctions of a Hermitian operator satisfying BCs form a complete set.

Proof of (1):

$$\mathcal{L} y_n + \lambda_n w y_n = 0$$

$$\mathcal{L} y_m + \lambda_m w y_m = 0$$

$$\int_a^b dx\, y_m^* \mathcal{L} y_n + \lambda_n \int_a^b dx\, w\, y_m^* y_n = 0$$

Since $\mathcal{L}$ is Hermitian,

$$\int_a^b dx\, y_n (\mathcal{L} y_m)^* + \lambda_n \int_a^b dx\, w\, y_m^* y_n = 0$$

$$-\int_a^b dx\, \lambda_m^* \, w\, y_m^* y_n + \lambda_n \int_a^b dx\, w\, y_m^* y_n = 0$$

$$\boxed{(\lambda_n - \lambda_m^*) \int_a^b dx\, w\, y_m^* y_n = 0}$$

If $m=n$ then

$$(\lambda_n - \lambda_n^*) \int_a^b dx\, |y_n|^2 w = 0$$

Since $w(x)$ is positive or at worst zero at a finite # of points, must have

$$\boxed{\lambda_n = \lambda_n^*} \Rightarrow \text{eigen value is real}$$

If $m \neq n$ and if $\lambda_m \neq \lambda_n$ must have

$$\boxed{\int_a^b dx\, w(x)\, y_n\, y_m^* = 0}$$

$\Rightarrow$ the eigen functions are orthogonal.

$\Rightarrow$ the weight function $w(x)$ must be included in the orthogonality relation.

What if $m \neq n$ but $\lambda_m = \lambda_n$?

$\Rightarrow$ degenerate eigenvalues

$\Rightarrow$ basis functions not necessarily orthogonal

<u>example</u>

$$\left(\frac{d^2}{dx^2} + k^2\right) y = 0$$

Consider interval $(0, 2\pi)$ with y periodic.
Eigenvalues $k_n = n = $ integer.

$\Rightarrow$ satisfies BC. $\quad y_n y_m^* \Big|_a^b = 0$

since periodic

$\Rightarrow$ For each value of n, have two eigenfunctions

$$y_n \sim e^{\pm inx}$$

$\Rightarrow$ an arbitrary combination

$$y_{n1} = a e^{inx} + b e^{-inx}$$

$$y_{n2} = c e^{inx} + d e^{-inx}$$

are not orthogonal but can force them to be orthogonal

$$\int_0^{2\pi} dx\, y_{n1}^* y_{n2} = 0 = \int_0^{2\pi} dx \left(a^* e^{-inx} + b^* e^{inx}\right) \otimes \left(c e^{inx} + d e^{-inx}\right)$$

$$= a^* c\, 2\pi + b^* d\, 2\pi = 0$$

$$c = -\frac{b^* d}{a^*}$$

Of course, we could have taken

$$y_{n1} = \sin nx$$
$$y_{n2} = \cos nx$$

$\Rightarrow$ for degenerate eigenvalues must force orthogonality since it is not automatic

Normalization

In general, we have

$$\int_a^b dx\, w\, |y_n|^2 = N_n^2$$

where N_n is a real number. We can define our functions

$$\hat{y}_n = \frac{y_n}{N_n}$$

so

$$\int_a^b dx\, w\, |\hat{y}_n|^2 = 1$$

Thus

$$\int_a^b dx\, w\, \hat{y}_m^* \hat{y}_n = \delta_{mn}$$

$\Rightarrow$ orthogonal and normalized $\Rightarrow$ orthonormal set