Analytical Methods

Boundary-value problems (II)

Part A – *General considerations*

- In the ***preceding*** we focused on ***inhomogeneous*** boundary-vale problems.

- In these problems - the *associated homogeneous* problem had only a ***trivial solution***.

Example

$$y'' + y = 1$$

$$y(0) = 0 \quad , y(\pi/2) = 0$$

$$\longrightarrow \quad \boxed{\varphi(x) = 1 - cos(x) - sin(x)}$$

- The *associated homogeneous* problem:

$$y'' + y = 0$$

$$y(0) = 0 \quad , y(\pi/2) = 0$$

$$\longrightarrow \quad \boxed{\varphi(x) = 0}$$

Eigenvalue problems

- In the following we focus on ***homogeneous*** boundary-vale problems.

A simple example

$$y'' + \lambda \cdot y = 0$$

$$y(0) = 0 \quad , y(1) = 0$$

$\lambda = 1$ → $\varphi(x) = 0$

Trivial solution

$\lambda_n = (n \cdot \pi)^2$ → $\varphi_n(x) = C \cdot \sin(n \cdot \pi \cdot x)$

*An **infinite** set of non-trivial solutions (arbitrary C)*

- These problems will have a ***free parameter*** λ.

- For certain λ values → ***non-trivial solutions*** **may** be obtained.

What λ values will produce non-trivial solutions ?

Example 1- (Regular B.C)

$$y'' + \lambda \cdot y = 0 \qquad (0 \le x \le 1)$$

$$y(0) = 0 \ , \quad y(1) + k \cdot y'(1) = 0 \qquad (k > 0)$$

$$\downarrow$$

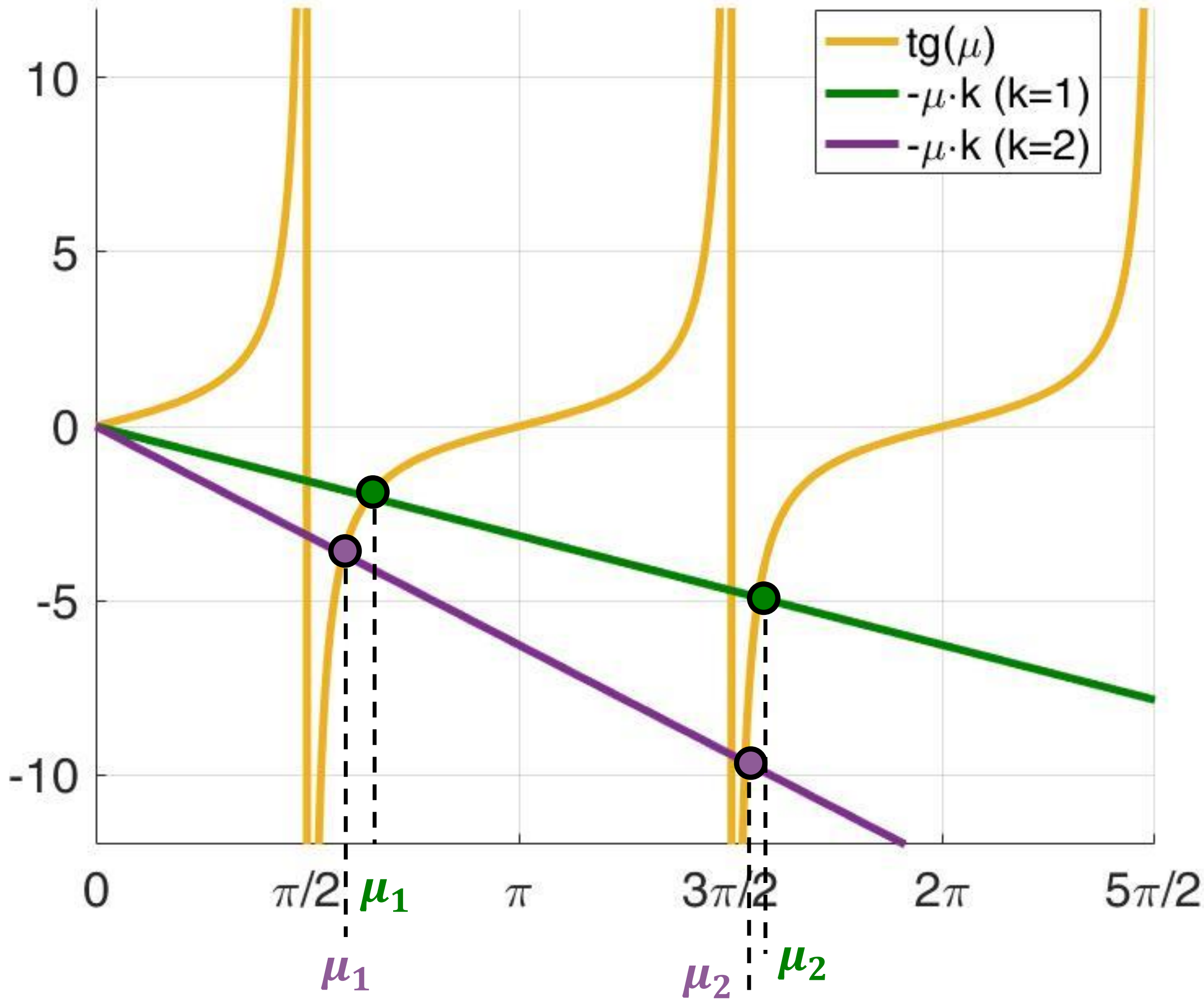
$$\boxed{\lambda_n = \mu_n^2}$$ ***eigenvalues***

$$\boxed{\varphi_n(x) = A_n \cdot \sin(\mu_n \cdot x)}$$ ***eigenfunctions***

$$\boxed{tan(\mu) = -\mu \cdot k}$$

$$\boxed{k = 1 \rightarrow \ \mu_1 = 2.03 \, , \mu_2 = 4.93 \ \ldots}$$

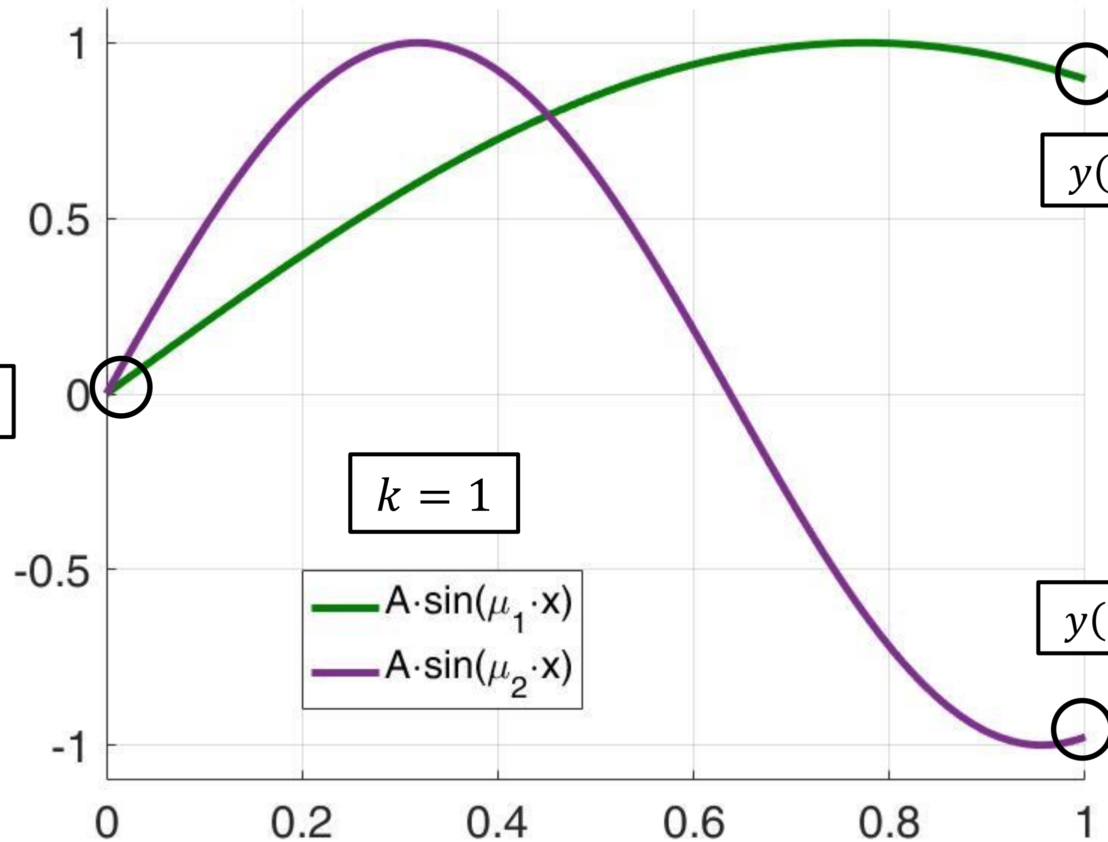
$$\boxed{tan(\mu) = -\mu \cdot k}$$



$$\boxed{\lambda_n = \mu_n^2}$$

$k = 1 \rightarrow \mu_1 = 2.03\,, \mu_2 = 4.93\ \ldots$

$$\boxed{\varphi_n(x) = A_n \cdot \sin(\mu_n \cdot x)}$$



$y(0) = 0$

$k = 1$

$y(1) + y'(1) = 0$

$y(1) + y'(1) = 0$

Example 2 (Periodic B.C.)

$$y'' + \lambda \cdot y = 0 \qquad (-\pi \le x \le \pi)$$

$$p(-\pi) = p(\pi) = 1 \qquad y(-\pi) = y(\pi) \quad , \quad y'(-\pi) = y'(\pi)$$

$$\downarrow$$

$$\boxed{\lambda_n = n^2}$$ ***eigenvalues***

$$\boxed{\varphi_n(x) = A_n \cdot \sin(n \cdot x)} \qquad \boxed{\varphi_n(x) = B_n \cdot \cos(n \cdot x)}$$ ***eigenfunctions***

Two eigenfunctions for each eigenvalue !!!!

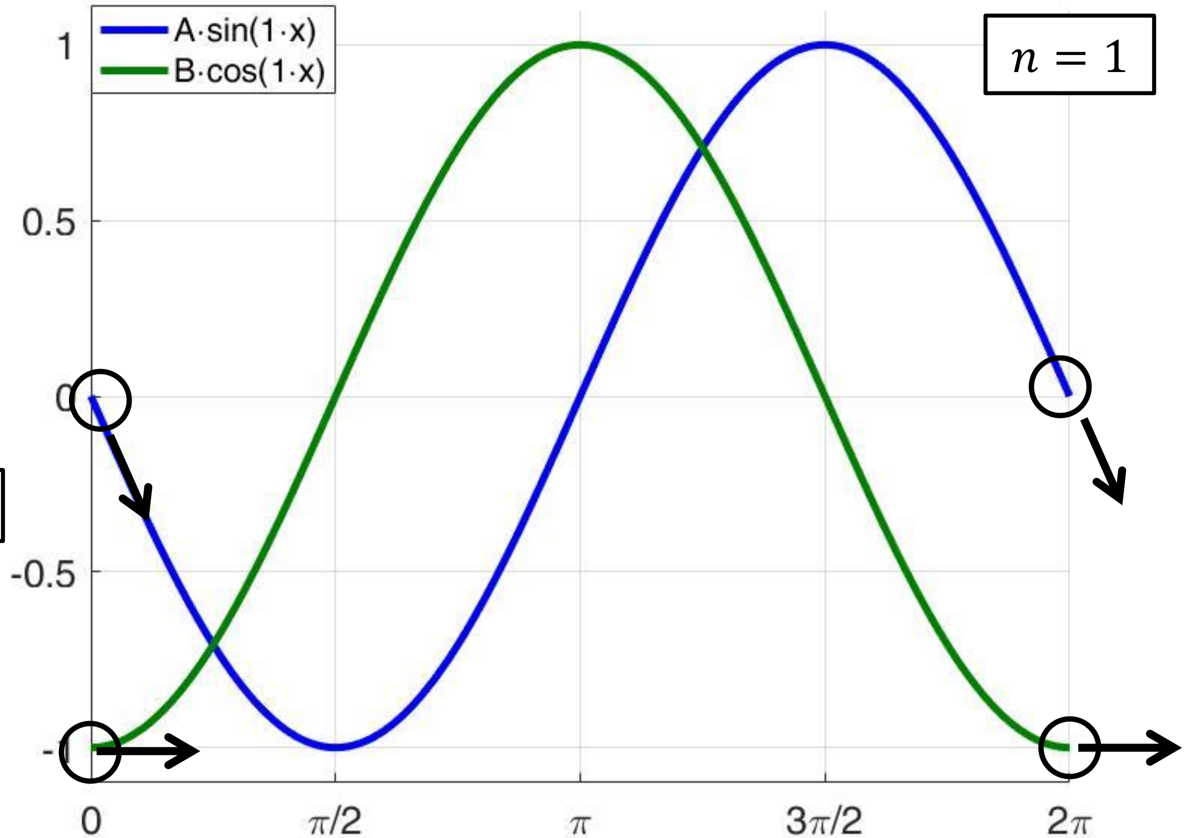
$$\lambda_n = n^2$$

$$\varphi_n(x) = A_n \cdot \sin(n \cdot x)$$

$$\varphi_n(x) = B_n \cdot \cos(n \cdot x)$$

$$y(-\pi) = y(\pi)$$

$$y'(-\pi) = y'(\pi)$$



Example 3 - Bessel's equation (Singular B.C.)

Friedrich Wilhelm Bessel

$$x^2 \cdot y'' + x \cdot y' + (\lambda \cdot x^2 - \nu^2) \cdot y = 0 \qquad (\nu \geq 0)$$

$$(0 < x \leq 1)$$

$$\lim_{x \to 0} y(x) < \infty \;\; ; \;\; p(x = 0) = 0$$

$$y(1) = 0$$

$$\downarrow$$

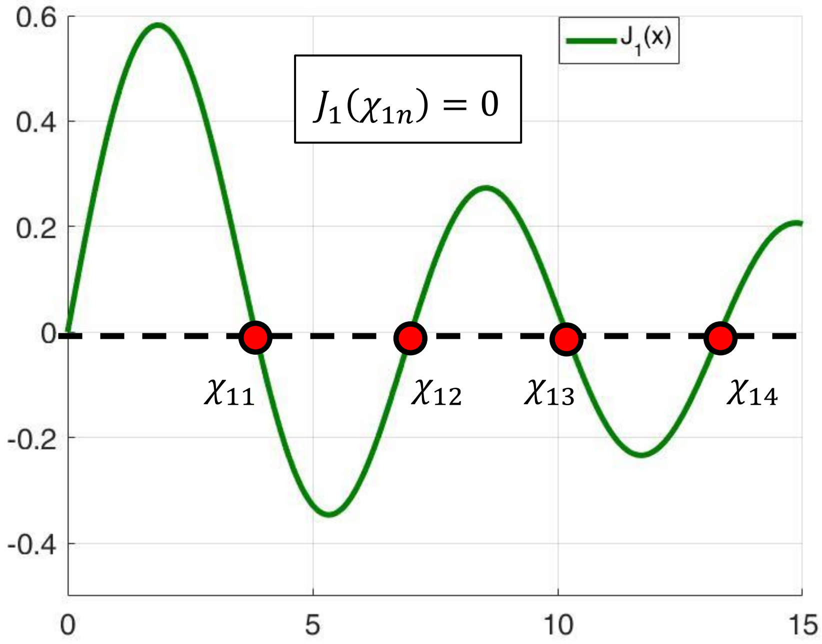
$x_{\nu n}$ - the n^{th} zero of Bessel equation of an order ν

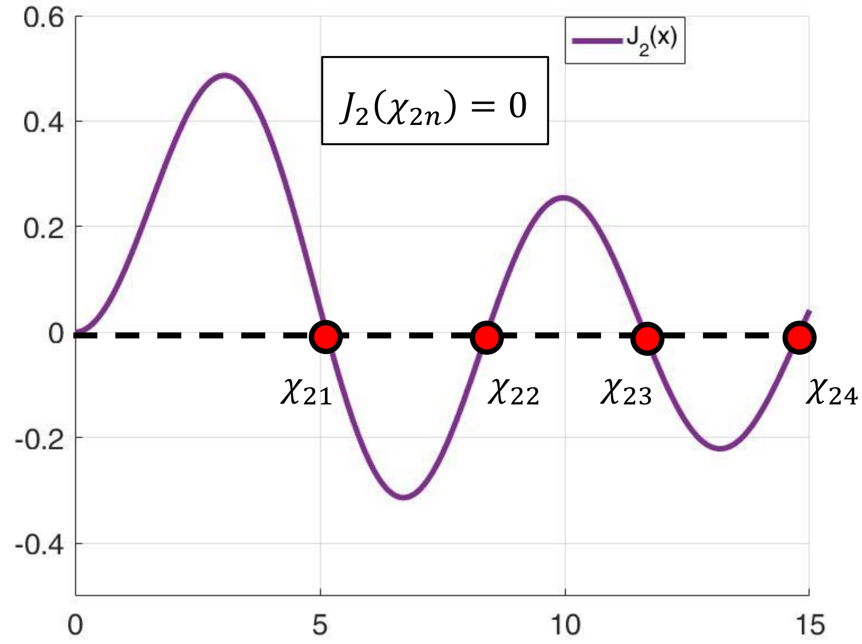
$$\boxed{\lambda_n = (x_{\nu n})^2}$$ **eigenvalues**

$$\boxed{\varphi_n(x) = A_n \cdot J_\nu(x_{\nu n} \cdot x)}$$ **eigenfunctions**

Reminder: Zeroes of Bessel functions

$$\boxed{J_\nu(\chi_{\nu n}) = 0 \quad (n = 1,2,3 \dots)}$$

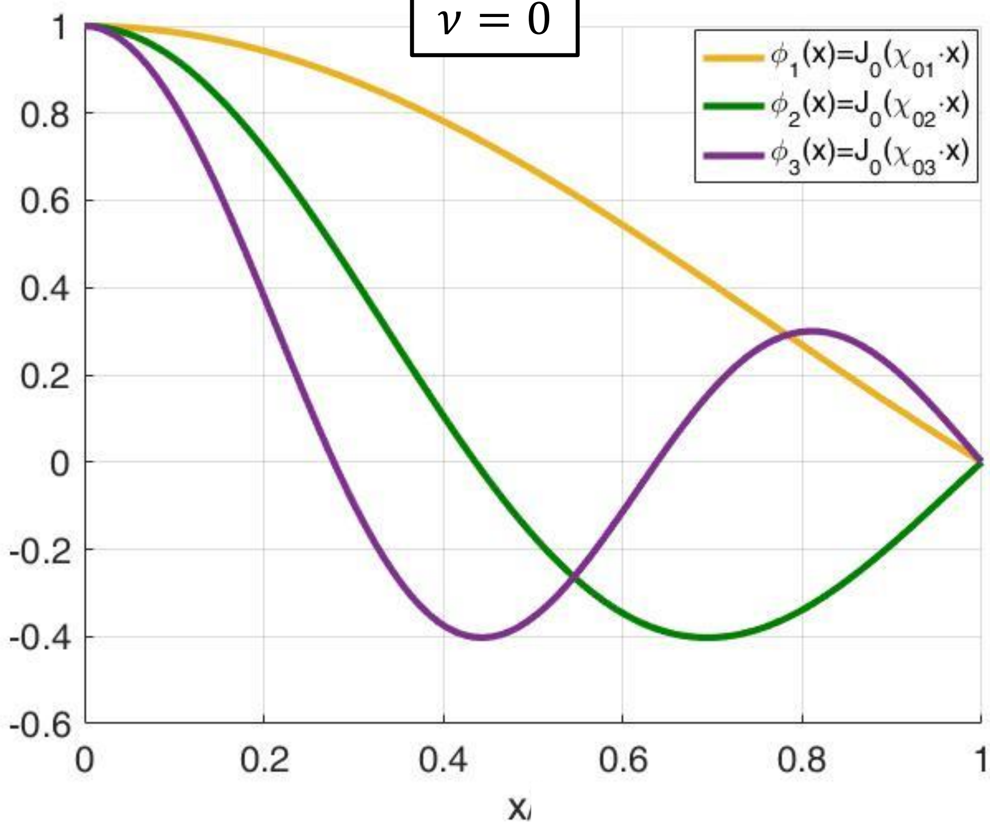




$$\boxed{\lambda_n = (x_{\nu n})^2}$$

$$\boxed{\varphi_n(x) = A_n \cdot J_\nu(x_{\nu n} \cdot x)}$$

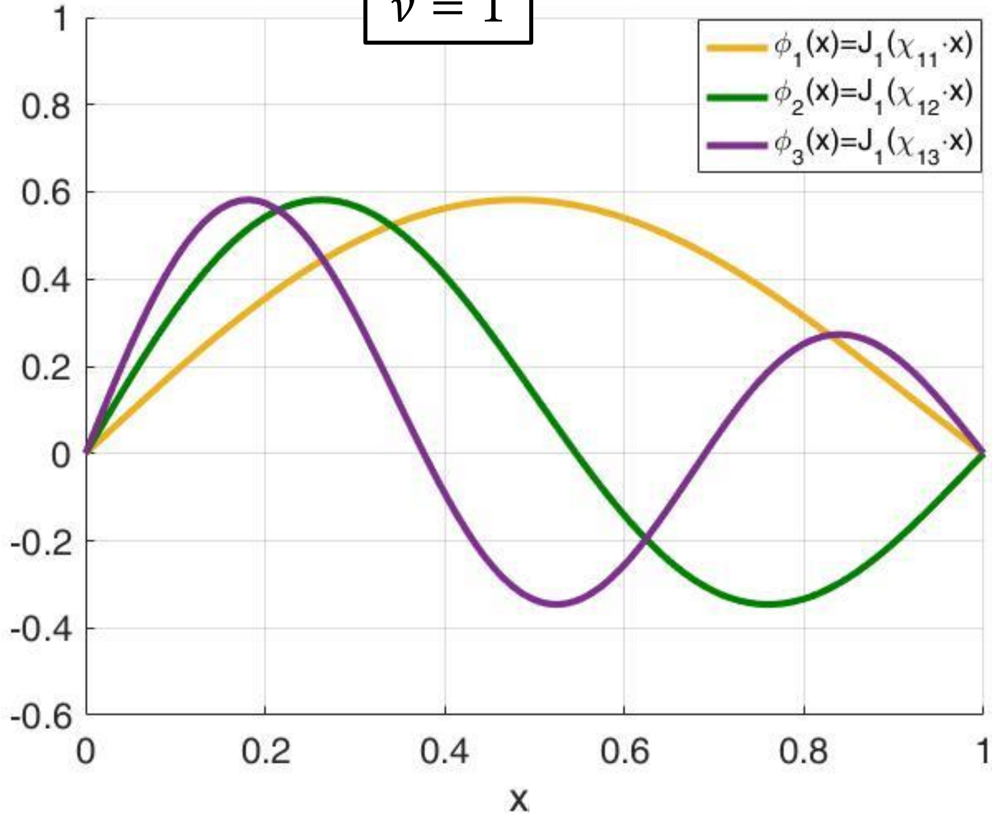
$$\boxed{\nu = 0}$$



$$\boxed{\lambda_n = (x_{\nu n})^2}$$

$$\boxed{\varphi_n(x) = A_n \cdot J_\nu(x_{\nu n} \cdot x)}$$

$$\boxed{\nu = 1}$$



Example 4 – Legendre equation (Singular B.C.)

Adrien-Marie Legendre

$$(1-x^2)\cdot y'' - 2x\cdot y' + \lambda\cdot y = 0 \qquad (-1 \le x \le 1)$$

$$\lim_{x\to -1} y(x) < \infty \;;\; p(x=-1) = 0$$

$$\lim_{x\to 1} y(x) < \infty \;;\; p(x=1) = 0$$

$$\downarrow$$

$(l = 0,1,2\ldots)$ $\boxed{\lambda_l = l\cdot(1+l)}$ ***eigenvalues***

$\boxed{\varphi_l(x) = A_l\cdot p_l(x)}$ ***eigenfunctions***

$P_l(x)$ - *Legendre polynomials*

(converge for $-1 \le x \le 1$)

The Legendre polynomials

$$l = 0 \longrightarrow P_0(x) = 1$$

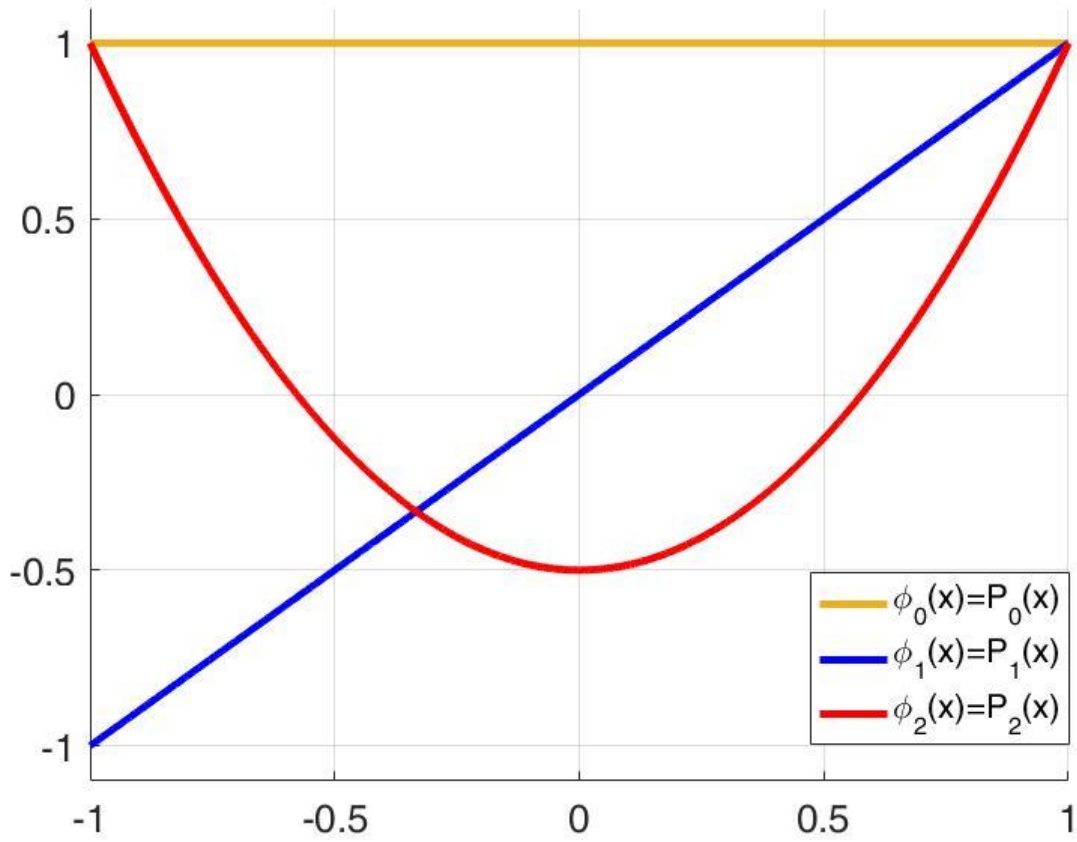
$$l = 1 \longrightarrow P_1(x) = x$$

$$l = 2 \longrightarrow P_2(x) = \frac{1}{2} \cdot (3x^2 - 1)$$

$$l = 3 \longrightarrow P_3(x) = \frac{1}{2} \cdot (5x^3 - 3x)$$

$$\boxed{\lambda_l = l \cdot (1 + l)}$$

$$\boxed{\varphi_l(x) = A_l \cdot p_l(x)}$$



Part B –Sturm-Liouville systems

Jacques Charles François Sturm

Joseph Liouville

(I) The Strum-Liouville system – eigenvalue problems

(1) The S-L equation

$$\boxed{\frac{d}{dx}\left(p(x)\cdot\frac{dy}{dx}\right)+\left(q(x)+\lambda\cdot s(x)\right)\cdot y=0}$$

Strum-Liouville equation

- The functions $p(x)$, $q(x)$ and $s(x)$ are real valued functions of x

- The *parameter* λ is ***independent*** of x

- Using the differential operator:

$$L=\tilde{L}=\frac{d}{dx}\left(p(x)\cdot\frac{d}{dx}\right)+q(x)$$

Strum-Liouville operator

- The equation takes the form of:

$$\boxed{L[y]+\lambda\cdot s(x)\cdot y=0}$$

$$\boxed{L[y] + \lambda \cdot s(x) \cdot y = 0} \qquad (a \le x \le b)$$

(2) The S-L boundary-conditions

$$\begin{cases} a_1 \cdot y(a) + a_2 \cdot y'(a) = 0 \\ b_1 \cdot y(b) + b_2 \cdot y'(b) = 0 \end{cases}$$

Regular S-L

$$\begin{cases} y(a) = y(b) \;\; ; \;\; y'(a) = y'(b) \\ p(x = a) = p(x = b) \end{cases}$$

Periodic S-L

$$\begin{cases} \lim_{x \to a} y(x) < \infty \;\; ; \;\; p(x = a) = 0 \\ b_1 \cdot y(b) + b_2 \cdot y'(b) = 0 \end{cases}$$

Singular S-L

*S-L systems are **self-adjoint** boundary-value problems !*

(3) The eigenvalue formulation

$$U_a[y] = 0 \qquad U_b[y] = 0$$

$$\boxed{L[y] = -\lambda \cdot s(x) \cdot y} \qquad (a \le x \le b)$$

- This problem ***always*** has a ***trivial solution***. $\boxed{\varphi(x) = 0}$

Are non-trivial solutions also exist ?

- Remember that λ is ***yet undetermined*** parameter…

Objective: We thus ***seek*** for the λ_n *parameters* and $\varphi_n(x)$ *solutions* – such that

$$\boxed{L[\varphi_n] = -\lambda_n \cdot s(x) \cdot \varphi_n} \longleftrightarrow \boxed{\varphi_n(x;\lambda_n) \neq 0}$$

$\downarrow$ *eigenvalues*

$\downarrow$ *eigenfunction*

Methodology – solution of S-L systems

Step 1: *Transform* the equation into S-L form and identify $p(x)$, $q(x)$ and $s(x)$

$$\frac{d}{dx}\left(p(x)\cdot\frac{dy}{dx}\right)+\left(q(x)+\lambda\cdot s(x)\right)\cdot y=0$$

(important for later…)

Step 2: *Find the general solution of the equation* (λ – yet unknown).

$$\varphi(x;\lambda)=A\cdot\varphi_1(x;\lambda)+B\cdot\varphi_2(x;\lambda)$$

Step 3: *Apply B.C.* and identify the set of λ *eigenvalues* that produce non-trivial solutions.

$$\lambda=\{\lambda_1,\lambda_2,\dots,\lambda_n\}$$

Step 4: Find the corresponding *eigenfunctions* to each λ_n (can be more than one)

$$\varphi_n(x;\lambda_n)\neq 0$$

(II) Characteristics of eigenvalues and eigenfunctions of S-L system

Theorem – regular S-L systems

$$\begin{cases} a_1 \cdot y(a) + a_2 \cdot y'(a) = 0 \\ b_1 \cdot y(b) + b_2 \cdot y'(b) = 0 \end{cases}$$

*A regular S-L system has an **infinite** **sequence** of **real** and **distinct** eigenvalues.*

$$\lambda_0 < \lambda_1 < \lambda_2 < \cdots$$

with

$$\lim_{n \to \infty} \lambda_n = \infty$$

*For each eigenvalue λ_n - the corresponding eigenfunction φ_n is **real** and **uniquely** determined.*

$$\lambda_n \leftrightarrow \varphi_n$$

*The eigenfunction φ_n has **exactly** $\mathbf{n}$ **zeros** in $a < x < b$.*

$$\begin{cases} y(a) = y(b) \;\; ; \;\; y'(a) = y'(b) \\ p(x=a) = p(x=b) \end{cases}$$

Theorem – periodic S-L systems

The eigenvalues of a periodic S-L system form a sequence:

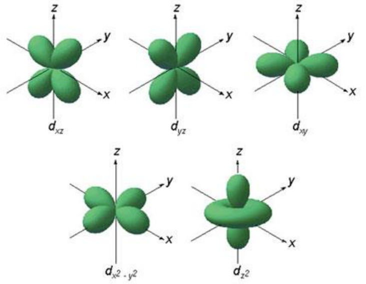
$$-\infty < \lambda_0 < \lambda_1 \le \lambda_2 \le \lambda_3 \le \cdots$$

There exists a unique eigenvalue λ_0 with a unique eigenfunction φ_0.

$$\lambda_0 \leftrightarrow \varphi_0$$

If $\lambda_{k+1} < \lambda_{k+2}$ then the eigenfunctions φ_{k+1} and φ_{k+2} are distinct.

$$\lambda_{k+1} \leftrightarrow \varphi_{k+1} \qquad \lambda_{k+2} \leftrightarrow \varphi_{k+2}$$



*If $\lambda_{k+1} = \lambda_{k+2}$ the the eigenfunctions φ_{k+1} and φ_{k+2} are yet **linear independent** – but share the same eigenvalue:*

$$\lambda_{k+1} \leftrightarrow \varphi_{k+1} \qquad \lambda_{k+1} \leftrightarrow \varphi_{k+2}$$

e.g. degenerated states in atomic orbitals

$$\begin{cases} \lim_{x \to a} y(x) < \infty \ ; \ p(x=a) = 0 \\ b_1 \cdot y(b) + b_2 \cdot y'(b) = 0 \end{cases}$$

A few comments - Singular S-L system

- The *eigenvalue* "***spectrum***" of a singular S-L system may be ***discrete*** and/or **continues**.

- For the ***discrete*** case, we have a set of eigenvalues and eigenfunctions – as before.

$$\lambda_0 < \lambda_1 \le \lambda_2 \le \lambda_3 \le \cdots \qquad\qquad \lambda_n \leftrightarrow \varphi_n(x)$$

- For the ***continues*** case, the eigenvalues λ take a certain ***range*** – generating a set of "two-variable" functions:

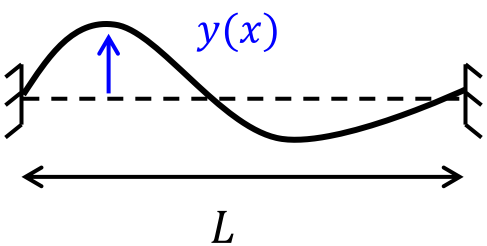
$$\lambda_i \le \lambda \le \lambda_j \qquad\qquad \lambda \leftrightarrow \varphi(x,\lambda)$$

Much less intuitive…

- Let's see this through an example....

Examples – Standing waves in a string

(1) Finite-length string (warm-up)



$$y'' + \lambda \cdot y = 0 \qquad (0 \le x \le L)$$

$$y(0) = 0 \quad , \quad y(L) = 0$$

- This is a ***regular*** S-L system – for which the general solution is:

$$\varphi(x) = A \cdot \sin(\kappa \cdot x) + B \cdot \cos(\kappa \cdot x) \qquad \lambda = \kappa^2$$

- Satisfying the B.C. produces:

$$y(0) = 0 \longrightarrow B = 0$$

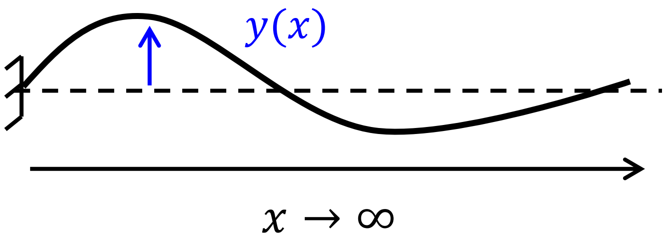
"wavenumber"

$$y(L) = 0 \longrightarrow \sin(\kappa \cdot L) = 0 \longrightarrow \kappa_n = n \cdot \frac{\pi}{L}$$

- The eigenfunctions and eigenvalues are thus:

$$\boxed{\varphi_n(x) = \sin(\kappa_n \cdot x)} \qquad \boxed{\lambda_n = \kappa_n^2 = \left(n \cdot \frac{\pi}{L}\right)^2} \qquad n = 1,2,\ldots$$

(2) A semi-infinite string ($L \to \infty$)



$$y'' + \lambda \cdot y = 0 \qquad (0 \le x < \infty)$$

$$y(0) = 0 \quad , \quad y(x \to \infty) = ?$$

- To obtain a ***singular*** S-L system, the B.C term at $x \to \infty$ must be:

$$\lim_{x\to\infty} y(x) < \infty$$ ✓ *Can be satisfied*

$$\lim_{x\to\infty} p(x) = 0$$ ✗ *Cannot be satisfied* $p(x) = 1$

- Thus it is a ***not well-defined singular*** S-L system – but yet an ***eigenvalue problem***

- Other techniques ***must*** be employed (integral transformations – *beyond our scope*…)

Any ideas for an "informal" alternative ???

Adaptation *of the finite-length solution for $L \to \infty$.*

- For the finite-length case we obtained:

$$\varphi_n(x) = \sin(\kappa_n \cdot x) \qquad \lambda_n = \kappa_n^2 = \left(n \cdot \frac{\pi}{L}\right)^2 \qquad n = 1,2,\ldots$$

- When taking $L \to \infty$, the eigenvalues λ_n approaches to a positive ***continues*** parameter (λ):

$$\lambda_n = \left(n \cdot \frac{\pi}{L}\right)^2 \longrightarrow 0 < \lambda$$

Eigenvalues range

- Similarly, the half-wavenumbers κ_n also approaches to a positive ***continues*** parameter (κ):

$$\kappa_n = \sqrt{\lambda_n} \longrightarrow 0 < \sqrt{\lambda} = \kappa$$

Wavenumber range

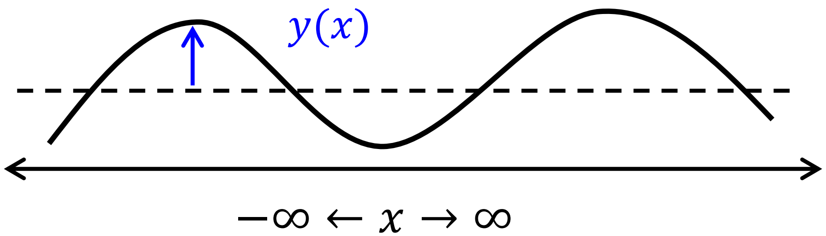
- The eigenfunction becomes a ***continues*** function of both x and κ:

$$\varphi_n(x) = \sin(\kappa_n \cdot x) \longrightarrow \varphi_\kappa(x) = \varphi(x,\kappa) = \sin(\kappa \cdot x)$$

*"**Descrete**" eigenfunction set*

*"**Continues**" eigenfunction set*

(3) An infinite string



$$y'' + \lambda \cdot y = 0 \qquad (-\infty \le x < \infty)$$

$$\lim_{x \to -\infty} y(x) < \infty, \quad \lim_{x \to \infty} y(x) < \infty$$

- This is also a ***not*** ***well-defined*** ***singular*** S-L system – but yet an ***eigenvalue problem***

- The ***general*** solution is:

$$\varphi(x) = A \cdot \sin(\kappa \cdot x) + B \cdot \cos(\kappa \cdot x) \qquad \lambda = \kappa^2$$

- As seen, a *non-trivial solution* is obtained for ***any*** κ value (eigenvalue) that is:

$$0 < k \in \mathcal{R}$$

Continues *eigenvalues* *range*

- Thus, each eigenvalue (κ) has ***two*** eigenfunctions:

$$\varphi_k(x) = \varphi(x, \kappa) = \sin(\kappa \cdot x) \qquad \psi_k(x) = \psi(x, \kappa) = \cos(\kappa \cdot x)$$

Continues
eigenfunction *sets*