



PHY 711 Classical Mechanics and Mathematical Methods

10-10:50 AM MWF in Olin 103


Discussion on Lecture 19 – Chap. 7 (F&W)

Solutions of differential equations

- 1. The wave equation – traveling wave solutions**
- 2. The wave equation – standing wave solutions**
- 3. The Sturm-Liouville equation**

Mid-term exams will be returned at the end of class.



14	Wed, 9/27/2023	Chap. 1	Scattering analysis	#13
15	Fri, 9/29/2023	Chap. 1	Scattering analysis	#14
16	Mon, 10/2/2023	Chap. 4	Small oscillations near equilibrium	
17	Wed, 10/4/2023	Chap. 4	Normal mode analysis	Mid term start
18	Fri, 10/6/2023	Chap. 4	Normal mode analysis	
22	Mon, 10/9/2023	Chap. 7	Normal modes of continuous string	
20	Wed, 10/11/2023		Review and summary	Mid term due
	Fri, 10/13/2023	Fall Break		
	21	Mon, 10/16/2023	Chap. 7	The wave and other partial differential equations #15
	22	Wed, 10/18/2023		
	23	Fri, 10/20/2023		
	24	Mon, 10/23/2023		
	25	Wed, 10/25/2023		
	26	Fri, 10/27/2023		
	27	Mon, 10/30/2023		

PHY 711 – Assignment #15

Assigned: 10/16/2023

Due: 10/23/2023 10/03/2022

Continue reading Chapter 7 in **Fetter and Walecka**.

1. Consider a one-dimensional traveling wave characterized by displacement $\mu(x, t)$ as a function of position x for $-\infty \leq x \leq \infty$ and time t for $0 \leq t \leq \infty$, is described by the wave equation:

$$\frac{\partial^2 \mu}{\partial t^2} - c^2 \frac{\partial^2 \mu}{\partial x^2} = 0, \quad (1)$$

where c denotes the wave speed. Find the functional form for the traveling wave $\mu(x, t)$ for each of these initial conditions.

- (a) At $t = 0$,

$$\mu(x, 0) = \frac{A}{\cosh(x)} \quad \text{and} \quad \frac{\partial \mu(x, 0)}{\partial t} = 0, \quad (2)$$

where A is a given wave amplitude.

- (b) At $t = 0$,

$$\mu(x, 0) = 0 \quad \text{and} \quad \frac{\partial \mu(x, 0)}{\partial t} = \frac{A \sinh(x)}{\cosh^2(x)}, \quad (3)$$

where A is a given wave speed amplitude.

PHYSICS AND CHEMISTRY

JOINT COLLOQUIUM

THURSDAY

OCTOBER 19TH, 2023

Molecular Photovoltaics and the Advent of Perovskite Solar Cells

Photovoltaic cells using molecular dyes, semiconductor quantum dots or perovskite pigments as light harvesters have emerged as credible contenders to conventional devices. Dye sensitized solar cells (DSCs) use a three-dimensional nanostructured junction for photovoltaic electricity production and currently reach a power conversion efficiency (PCE) of 15.2 % in full sunlight and over 30 % in ambient light. They possess unique practical advantages in terms of particularly high effective electricity production from ambient light, ease of manufacturing, flexibility and transparency, bifacial light harvesting, and aesthetic appeal, which have fostered large scale industrial production and commercial applications. They served as a launch pad for perovskite solar cells (PSCs) which are presently being intensively investigated as one of the most promising future PV technologies, the PCE of solution processed laboratory cells having currently reached 25.7%. Present research focuses on their scale up to as well as ascertaining their long-term operational stability. This lecture will cover the most recent findings in these revolutionary photovoltaic domains.



Michael Grätzel

EPFL
Switzerland

Note that lecture location is in
Salem Hall →

4 pm - Salem 012

Refreshments served prior to seminar

Reminder -- this is a good time to be choosing your project topics –

Project

The purpose of this assignment is to provide an opportunity for you to study a topic of your choice in greater depth. The general guideline for your choice of project is that it should have something to do with classical mechanics, and there should be some degree of analytic or numerical computation associated with the project. The completed project will include a short write-up and a presentation to the class. You may design your own project or use one of the following list (which will be updated throughout the term).

- Explain the details of a homework problem that was assigned or one you design, including the basic principles and the solution methods and results.
- Consider a scattering experiment in which you specify the spherically symmetric interaction potential $V(r)$. Write a computer program (using your favorite language) to evaluate the scattering cross section for your system. (Depending on your choice, you may wish to present your results either in the center-of-mass or lab frames of reference.)
- Consider the Foucault Pendulum. Analyze the equations of motion including both the horizontal and vertical motions. You can either solve the equations exactly or use perturbation theory. Compare the effects of the vertical motion to the effects of air friction.
- Consider a model system of 2 or more interacting particles with appropriate initial conditions, using numerical methods to find out how the system evolves in time and space. For few particles and special initial conditions this approach can be used to explore orbital mechanics. For many particles and random initial conditions, this approach can be used to explore statistical mechanics via molecular dynamics simulations.
- Examine the normal modes of vibration for a model system with 3 or more masses in 2 or 3 dimensions.
- Analyze the soliton equations beyond what was covered in class.



One-dimensional wave equation

representing longitudinal or transverse displacements as a function of x and t , an example of a partial differential equation --

Traveling wave solutions thanks to D'Alembert --

For the displacement function, $\mu(x,t)$, the wave equation has the form:

$$\frac{\partial^2 \mu}{\partial t^2} - c^2 \frac{\partial^2 \mu}{\partial x^2} = 0$$

Note that for any function $f(q)$ or $g(q)$:

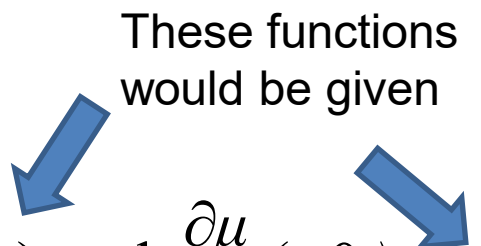
$$\mu(x,t) = f(x - ct) + g(x + ct)$$

satisfies the wave equation.

Initial value traveling wave solutions $\mu(x,t)$ to the wave equation; attributed to D'Alembert:

$$\frac{\partial^2 \mu}{\partial t^2} - c^2 \frac{\partial^2 \mu}{\partial x^2} = 0 \quad \text{where } \mu(x,0) = \varphi(x) \text{ and } \frac{\partial \mu}{\partial t}(x,0) = \psi(x)$$

These functions would be given



Assume:

$$\mu(x,t) = f(x-ct) + g(x+ct)$$

then: $\mu(x,0) = \varphi(x) = f(x) + g(x)$

$$\frac{\partial \mu}{\partial t}(x,0) = \psi(x) = -c \left(\frac{df(x)}{dx} - \frac{dg(x)}{dx} \right)$$

$$\Rightarrow f(x) - g(x) = -\frac{1}{c} \int^x \psi(x') dx'$$

Solution -- continued: $\mu(x,t) = f(x-ct) + g(x+ct)$

then: $\mu(x,0) = \phi(x) = f(x) + g(x)$

$$\frac{\partial \mu}{\partial t}(x,0) = \psi(x) = -c \left(\frac{df(x)}{dx} - \frac{dg(x)}{dx} \right)$$

$$\Rightarrow f(x) - g(x) = -\frac{1}{c} \int^x \psi(x') dx'$$

For each x , find $f(x)$ and $g(x)$:

$$f(x) = \frac{1}{2} \left(\phi(x) - \frac{1}{c} \int^x \psi(x') dx' \right)$$

$$g(x) = \frac{1}{2} \left(\phi(x) + \frac{1}{c} \int^x \psi(x') dx' \right)$$

$$\Rightarrow \mu(x,t) = \frac{1}{2} (\phi(x-ct) + \phi(x+ct)) + \frac{1}{2c} \int_{x-ct}^{x+ct} \psi(x') dx'$$

Checking that D'Alembert's solution solves the wave equation:

$$\frac{\partial^2 \mu}{\partial t^2} - c^2 \frac{\partial^2 \mu}{\partial x^2} = 0$$

$$\mu(x, t) = \frac{1}{2}(\varphi(x - ct) + \varphi(x + ct)) + \frac{1}{2c} \int_{x-ct}^{x+ct} \psi(x') dx'$$

$$\frac{\partial \mu(x, t)}{\partial x} = \frac{1}{2}(\varphi'(x - ct) + \varphi'(x + ct)) + \frac{1}{2c}(\psi(x - ct) + \psi(x + ct))$$

$$\frac{\partial^2 \mu(x, t)}{\partial x^2} = \frac{1}{2}(\varphi''(x - ct) + \varphi''(x + ct)) + \frac{1}{2c}(\psi'(x - ct) + \psi'(x + ct))$$

$$\frac{\partial \mu(x, t)}{\partial t} = \frac{c}{2}(-\varphi'(x - ct) + \varphi'(x + ct)) + \frac{c}{2c}(-\psi(x - ct) + \psi(x + ct))$$

$$\frac{\partial^2 \mu(x, t)}{\partial t^2} = \frac{c^2}{2}(\varphi''(x - ct) + \varphi''(x + ct)) + \frac{c^2}{2c}(\psi'(x - ct) + \psi'(x + ct))$$

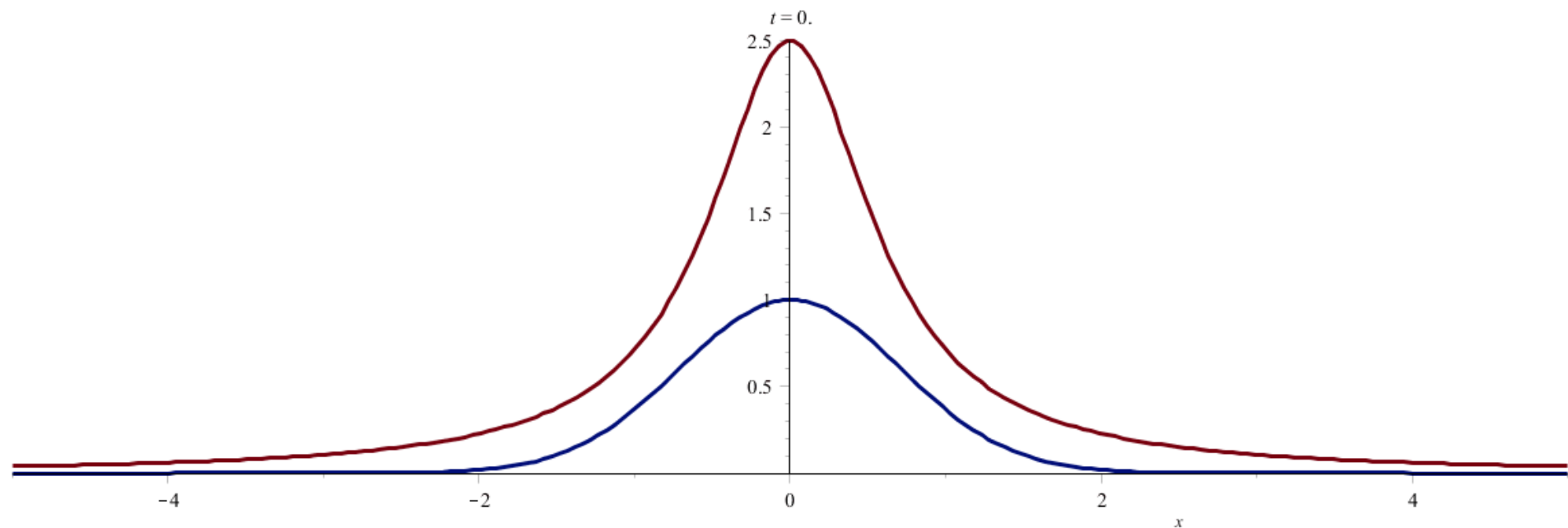
Here we have assumed that $\varphi(u)$ and $\psi(u)$ are continuous functions and

$$\varphi'(u) \equiv \frac{d\varphi(u)}{du}, \quad \varphi''(u) \equiv \frac{d^2\varphi(u)}{du^2}, \quad \text{etc.}$$

Example:

$$\frac{\partial^2 \mu}{\partial t^2} - c^2 \frac{\partial^2 \mu}{\partial x^2} = 0 \quad \text{where } \mu(x,0) = e^{-x^2/\sigma^2} \text{ and } \frac{\partial \mu}{\partial t}(x,0) = 0$$

$$\Rightarrow \mu(x,t) = \frac{1}{2} \left(e^{-(x+ct)^2/\sigma^2} + e^{-(x-ct)^2/\sigma^2} \right)$$

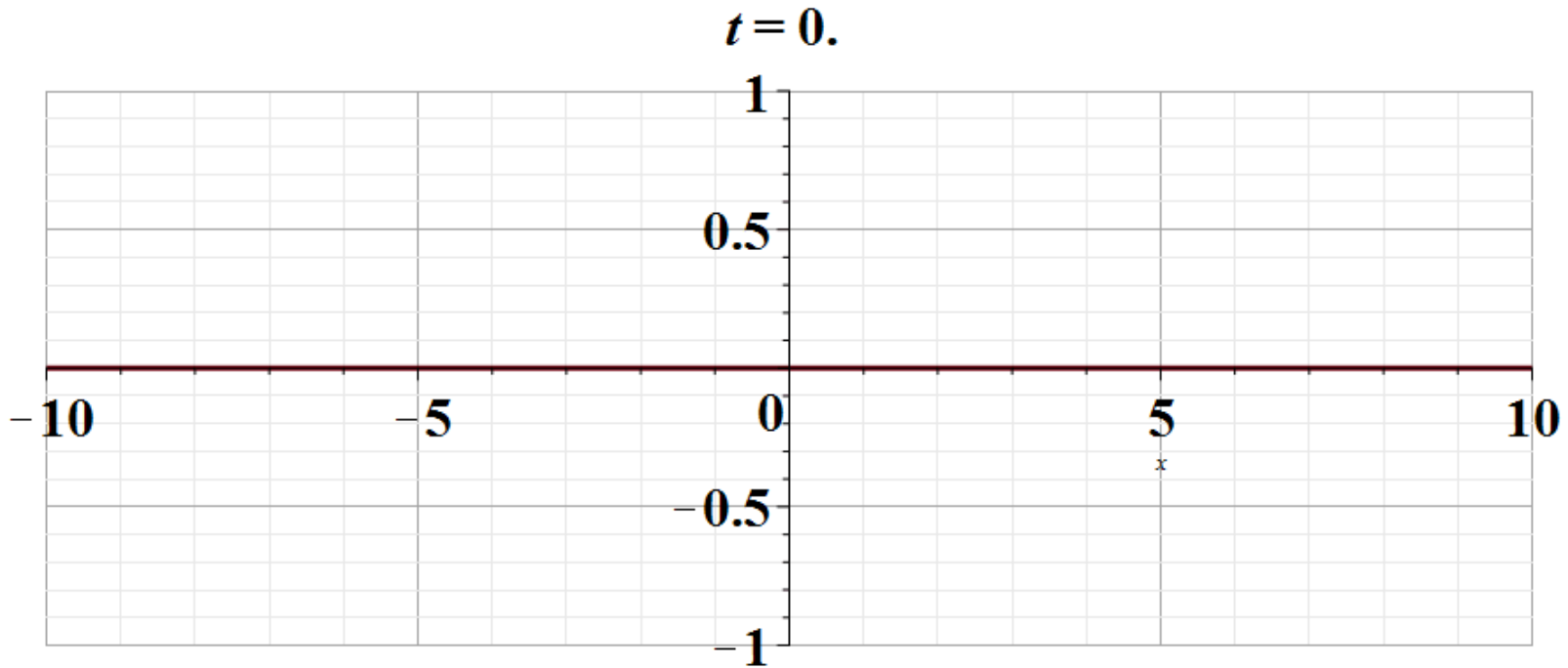


Example:

$$\frac{\partial^2 \mu}{\partial t^2} - c^2 \frac{\partial^2 \mu}{\partial x^2} = 0 \quad \text{where } \mu(x,0) = 0 \quad \text{and} \quad \frac{\partial \mu}{\partial t}(x,0) = -\frac{2x}{\sigma^2} e^{-x^2/\sigma^2}$$

$$\Rightarrow \mu(x,t) = \frac{1}{2c} \left(e^{-(x+ct)^2/\sigma^2} - e^{-(x-ct)^2/\sigma^2} \right)$$

$$\text{Note that } \frac{\partial \mu(x,t)}{\partial t} = -\frac{1}{\sigma^2} \left((x+ct)e^{-(x+ct)^2/\sigma^2} + (x-ct)e^{-(x-ct)^2/\sigma^2} \right)$$



Other types of solutions to the wave equation:

$$\frac{\partial^2 \mu}{\partial t^2} - c^2 \frac{\partial^2 \mu}{\partial x^2} = 0$$

Note that because of the way that the equation is written, it is possible to find "separable" solutions of the form

$$\mu(x, t) = X(x)T(t)$$

or more generally, a linear combination of separable solutions:

$$\mu(x, t) = \sum_n X_n(x)T_n(t)$$

Separable solutions to the wave equation:

$$\frac{\partial^2 \mu}{\partial t^2} - c^2 \frac{\partial^2 \mu}{\partial x^2} = 0 \quad \text{for} \quad \mu(x, t) = X(x)T(t)$$

$$\Rightarrow \frac{1}{X(x)} \frac{d^2 X(x)}{dx^2} = \frac{1}{c^2 T(t)} \frac{d^2 T(t)}{dt^2}$$

For example, suppose the time function is harmonic in time with frequency ω : $T(t) = \cos(\omega t + \eta)$

Then the spacial function must satisfy the ordinary differential equation:

$$\frac{d^2 X(x)}{dx^2} = -\frac{\omega^2}{c^2} X(x)$$

$$\Rightarrow X(x) = A \sin(kx + \nu) \quad \text{where} \quad k = \frac{\omega}{c}$$

It is often the case, there are boundary values specified for $X(x)$.

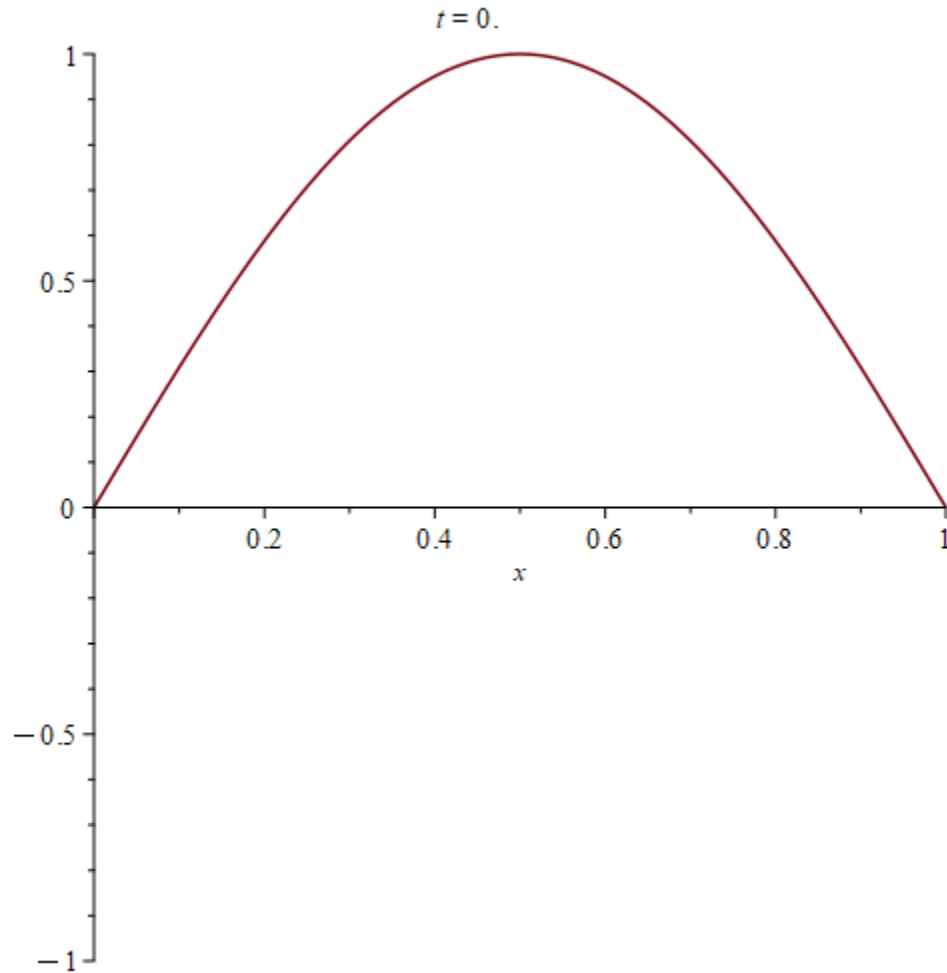
For example, suppose $X(0) = 0$ and $X(a) = 0$ — —

$$A \sin(kx) \Big|_{x=0} = 0 \quad A \sin(kx) \Big|_{x=a} = 0$$

$$\Rightarrow k = \frac{n\pi x}{a} \quad \text{for } n = 0, 1, 2, \dots$$

$$\Rightarrow X(x) = A \sin\left(\frac{n\pi x}{a}\right) \quad \text{and } \omega = \frac{n\pi c}{a}$$

Standing wave -- $\mu(x, t) = A \sin\left(\frac{n\pi x}{a}\right) \cos\left(\frac{n\pi ct}{a}\right)$



How are the traveling wave and standing wave solutions to the wave equations related?

- A. They are exactly the same
- B. They are not related
- C. ???

The wave equation and related linear PDE's

One dimensional wave equation for $\mu(x,t)$:

$$\frac{\partial^2 \mu}{\partial t^2} - c^2 \frac{\partial^2 \mu}{\partial x^2} = 0 \quad \text{where } c^2 = \frac{\tau}{\sigma}$$

Generalization for spatially dependent tension and mass density plus an extra potential energy density:

$$\sigma(x) \frac{\partial^2 \mu(x,t)}{\partial t^2} - \frac{\partial}{\partial x} \left(\tau(x) \frac{\partial \mu(x,t)}{\partial x} \right) + v(x) \mu(x,t) = 0$$

Factoring time and spatial variables:

$$\mu(x,t) = \phi(x) \cos(\omega t + \alpha)$$

Sturm-Liouville equation for spatial function $\phi(x)$:

$$-\frac{d}{dx} \left(\tau(x) \frac{d\phi(x)}{dx} \right) + v(x) \phi(x) = \omega^2 \sigma(x) \phi(x)$$



Linear second-order ordinary differential equations Sturm-Liouville equations

Inhomogenous problem: $\left(-\frac{d}{dx} \tau(x) \frac{d}{dx} + v(x) - \lambda \sigma(x) \right) \varphi(x) = F(x)$

given functions

applied force

solution to be determined

When applicable, it is assumed that the form of the applied force is known.

Homogenous problem: $F(x)=0$

Examples of Sturm-Liouville eigenvalue equations --

$$\left(-\frac{d}{dx} \tau(x) \frac{d}{dx} + v(x) - \lambda \sigma(x) \right) \varphi(x) = 0$$

Bessel functions: $0 \leq x < \infty$

$$\tau(x) = -x \quad v(x) = x \quad \sigma(x) = \frac{1}{x} \quad \lambda = \nu^2 \quad \varphi(x) = J_\nu(x)$$

Legendre functions: $-1 \leq x \leq 1$

$$\tau(x) = -(1-x^2) \quad v(x) = 0 \quad \sigma(x) = 1 \quad \lambda = l(l+1) \quad \varphi(x) = P_l(x)$$

Fourier functions: $0 \leq x \leq 1$

$$\tau(x) = 1 \quad v(x) = 0 \quad \sigma(x) = 1 \quad \lambda = n^2 \pi^2 \quad \varphi(x) = \sin(n\pi x)$$

Solution methods of Sturm-Liouville equations

(assume all functions and constants are real):

$$\text{Homogenous problem: } \left(-\frac{d}{dx} \tau(x) \frac{d}{dx} + v(x) - \lambda \sigma(x) \right) \phi_0(x) = 0$$

$$\text{Inhomogenous problem: } \left(-\frac{d}{dx} \tau(x) \frac{d}{dx} + v(x) - \lambda \sigma(x) \right) \phi(x) = F(x)$$

Eigenfunctions:

$$\left(-\frac{d}{dx} \tau(x) \frac{d}{dx} + v(x) \right) f_n(x) = \lambda_n \sigma(x) f_n(x)$$

$$\text{Orthogonality of eigenfunctions: } \int_a^b \sigma(x) f_n(x) f_m(x) dx = \delta_{nm} N_n,$$

$$\text{where } N_n \equiv \int_a^b \sigma(x) (f_n(x))^2 dx.$$

Completeness of eigenfunctions:

$$\sigma(x) \sum \frac{f_n(x) f_n(x')}{N_n} = \delta(x - x')$$

Why all of the fuss about eigenvalues and eigenvectors?

- a. They are sometimes useful in finding solutions to differential equations
- b. Not all eigenfunctions have analytic forms.
- c. It is possible to solve a differential equation without the use of eigenfunctions.
- d. Eigenfunctions have some useful properties.

Comment on orthogonality of eigenfunctions

$$\left(-\frac{d}{dx} \tau(x) \frac{d}{dx} + v(x) \right) f_n(x) = \lambda_n \sigma(x) f_n(x)$$

$$\left(-\frac{d}{dx} \tau(x) \frac{d}{dx} + v(x) \right) f_m(x) = \lambda_m \sigma(x) f_m(x)$$

$$\begin{aligned} f_m(x) \left(-\frac{d}{dx} \tau(x) \frac{d}{dx} + v(x) \right) f_n(x) - f_n(x) \left(-\frac{d}{dx} \tau(x) \frac{d}{dx} + v(x) \right) f_m(x) \\ = (\lambda_n - \lambda_m) \sigma(x) f_n(x) f_m(x) \end{aligned}$$

$$-\frac{d}{dx} \left(f_m(x) \tau(x) \frac{df_n(x)}{dx} - f_n(x) \tau(x) \frac{df_m(x)}{dx} \right) = (\lambda_n - \lambda_m) \sigma(x) f_n(x) f_m(x)$$

Comment on orthogonality of eigenfunctions -- continued

$$-\frac{d}{dx} \left(f_m(x) \tau(x) \frac{df_n(x)}{dx} - f_n(x) \tau(x) \frac{df_m(x)}{dx} \right) = (\lambda_n - \lambda_m) \sigma(x) f_n(x) f_m(x)$$

Now consider integrating both sides of the equation in the interval

$a \leq x \leq b$:

$$-\left(f_m(x) \tau(x) \frac{df_n(x)}{dx} - f_n(x) \tau(x) \frac{df_m(x)}{dx} \right) \Big|_a^b = (\lambda_n - \lambda_m) \int_a^b dx \sigma(x) f_n(x) f_m(x)$$



Vanishes for various boundary conditions
at $x=a$ and $x=b$



Comment on orthogonality of eigenfunctions -- continued

$$-\left(f_m(x)\tau(x)\frac{df_n(x)}{dx} - f_n(x)\tau(x)\frac{df_m(x)}{dx} \right) \Big|_a^b = (\lambda_n - \lambda_m) \int_a^b dx \sigma(x) f_n(x) f_m(x)$$

Possible boundary values for Sturm-Liouville equations:

1. $f_m(a) = f_m(b) = 0$

2. $\tau(x)\frac{df_m(x)}{dx} \Big|_a = \tau(x)\frac{df_m(x)}{dx} \Big|_b = 0$

3. $f_m(a) = f_m(b)$ and $\frac{df_m(a)}{dx} = \frac{df_m(b)}{dx}$

In any of these cases, we can conclude that:

$$\int_a^b dx \sigma(x) f_n(x) f_m(x) = 0 \text{ for } \lambda_n \neq \lambda_m$$



Comment on “completeness”

It can be shown that for any reasonable function $h(x)$, defined within the interval $a < x < b$, we can expand that function as a linear combination of the eigenfunctions $f_n(x)$

$$h(x) \approx \sum_n C_n f_n(x),$$

where
$$C_n = \frac{1}{N_n} \int_a^b \sigma(x') h(x') f_n(x') dx'.$$

These ideas lead to the notion that the set of eigenfunctions $f_n(x)$ form a “complete” set in the sense of “spanning” the space of all functions in the interval $a < x < b$, as summarized by the statement:

$$\sigma(x) \sum_n \frac{f_n(x) f_n(x')}{N_n} = \delta(x - x').$$



Comment on “completeness” -- continued

$$h(x) \approx \sum_n C_n f_n(x),$$

$$\text{where } C_n = \frac{1}{N_n} \int_a^b \sigma(x') h(x') f_n(x') dx'.$$

Consider the squared error of the expansion:

$$\epsilon^2 = \int_a^b dx \sigma(x) \left(h(x) - \sum_n C_n f_n(x) \right)^2$$

ϵ^2 can be minimized:

$$\frac{\partial \epsilon^2}{\partial C_m} = 0 = -2 \int_a^b dx \sigma(x) \left(h(x) - \sum_n C_n f_n(x) \right) f_m(x)$$

$$\Rightarrow C_m = \frac{1}{N_m} \int_a^b dx \sigma(x) h(x) f_m(x)$$