

**PHY 711 Classical Mechanics and  
Mathematical Methods  
10-10:50 AM MWF in Olin 103**

**Notes on Lecture 21 – Chap. 7 (F&W)**

**Solutions of differential equations**

- 1. Green's function solution methods based on eigenfunction expansions**
- 2. Green's function solution methods based on solutions of the homogeneous equations**

10/15/2021

PHY 711 Fall 2021 -- Lecture 21

1

In this lecture, we will continue our discussion of one dimensional ordinary differential equations.



Review – Sturm-Liouville equations defined over a range of  $x$ .

$$\text{Homogenous problem: } \left( -\frac{d}{dx} \tau(x) \frac{d}{dx} + v(x) - \lambda \sigma(x) \right) \varphi_0(x) = 0$$

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

Eigenfunctions:

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

Note that, because Sturm-Liouville operator is Hermitian, the eigenvalues are real and the eigenfunctions are orthogonal. In the last lecture, we argued that the eigenfunctions form a “complete” set over the range of  $x$  defined for the particular system.

10/15/2021

PHY 711 Fall 2021 -- Lecture 21

3

Review of the class problems considered.

## Eigenvalues and eigenfunctions of Sturm-Liouville equations

In the domain  $a \leq x \leq b$ :

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

Alternative boundary conditions; 1.  $f_m(a) = f_m(b) = 0$

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

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

Properties:

Eigenvalues  $\lambda_n$  are real

Eigenfunctions are orthogonal:  $\int_a^b \sigma(x) f_n(x) f_m(x) dx = \delta_{nm} N_n$ ,

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

10/15/2021

PHY 711 Fall 2021 -- Lecture 21

4

General properties.

### Variation approximation to lowest eigenvalue

In general, there are several techniques to determine the eigenvalues  $\lambda_n$  and eigenfunctions  $f_n(x)$ . When it is not possible to find the "exact" functions, there are several powerful approximation techniques. For example, the lowest eigenvalue can be approximated by minimizing the function

$$\lambda_0 \leq \frac{\langle \tilde{h} | S | \tilde{h} \rangle}{\langle \tilde{h} | \sigma | \tilde{h} \rangle}, \quad S(x) \equiv -\frac{d}{dx} \tau(x) \frac{d}{dx} + v(x)$$

where  $\tilde{h}(x)$  is a variable function which satisfies the correct boundary values. The "proof" of this inequality is based on the notion that  $\tilde{h}(x)$  can in principle be expanded in terms of the (unknown) exact eigenfunctions  $f_n(x)$ :

$$\tilde{h}(x) = \sum_n C_n f_n(x), \quad \text{where the coefficients } C_n \text{ can be}$$

assumed to be real.

10/15/2021

PHY 711 Fall 2021 -- Lecture 21

5

Comment on the Raleigh-Ritz approximation for the lowest eigenvalues.

Estimation of the lowest eigenvalue – continued:

From the eigenfunction equation, we know that

$$S(x)\tilde{h}(x) = S(x) \sum_n C_n f_n(x) = \sum_n C_n \lambda_n \sigma(x) f_n(x).$$

It follows that:

$$\langle \tilde{h} | S | \tilde{h} \rangle = \int_a^b \tilde{h}(x) S(x) \tilde{h}(x) dx = \sum_n |C_n|^2 N_n \lambda_n.$$

It also follows that:

$$\langle \tilde{h} | \sigma | \tilde{h} \rangle = \int_a^b \tilde{h}(x) \sigma(x) \tilde{h}(x) dx = \sum_n |C_n|^2 N_n,$$

$$\text{Therefore } \frac{\langle \tilde{h} | S | \tilde{h} \rangle}{\langle \tilde{h} | \sigma | \tilde{h} \rangle} = \frac{\sum_n |C_n|^2 N_n \lambda_n}{\sum_n |C_n|^2 N_n} \geq \lambda_0.$$

10/15/2021

PHY 711 Fall 2021 -- Lecture 21

6

Proof of the Rayleigh-Ritz theorem.

Rayleigh-Ritz method of estimating the lowest eigenvalue

$$\lambda_0 \leq \frac{\langle \tilde{h} | S | \tilde{h} \rangle}{\langle \tilde{h} | \sigma | \tilde{h} \rangle},$$

Example:  $-\frac{d^2}{dx^2} f_n(x) = \lambda_n f_n(x)$  with  $f_n(0) = f_n(a) = 0$

trial function  $f_{\text{trial}}(x) = x(x - a)$

Exact value of  $\lambda_0 = \frac{\pi^2}{a^2} = \frac{9.869604404}{a^2}$

Raleigh-Ritz estimate:  $\frac{\langle x(a-x) | -\frac{d^2}{dx^2} | x(a-x) \rangle}{\langle x(a-x) | x(a-x) \rangle} = \frac{10}{a^2}$

Review of example from last lecture.

Rayleigh-Ritz method of estimating the lowest eigenvalue

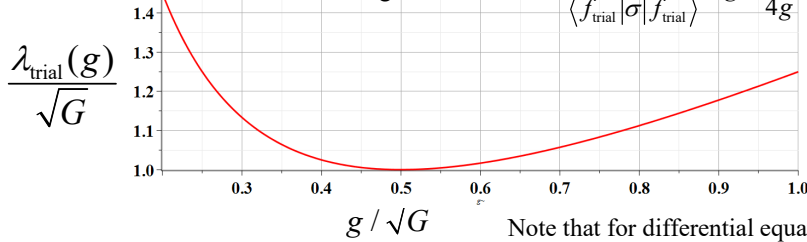
$$\lambda_0 \leq \frac{\langle \tilde{h} | S | \tilde{h} \rangle}{\langle \tilde{h} | \sigma | \tilde{h} \rangle},$$

Another example – this time with a variable parameter

Example:  $-\frac{d^2 f_n(x)}{dx^2} + Gx^2 f_n(x) = \lambda_n f_n(x)$  with  $f_n(-\infty) = f_n(\infty) = 0$

trial function  $f_{\text{trial}}(x) = e^{-gx^2}$

Raleigh-Ritz estimate:  $\frac{\langle f_{\text{trial}} | S | f_{\text{trial}} \rangle}{\langle f_{\text{trial}} | \sigma | f_{\text{trial}} \rangle} = g + \frac{G}{4g} \equiv \lambda_{\text{trial}}(g)$



$g_0 = \frac{1}{2} \sqrt{G}$      $\lambda_{\text{trial}}(g_0) = \sqrt{G}$

Note that for differential equation of the Schoedinger equation of the harmonic oscillator:

$\sqrt{G} = \frac{m\omega}{\hbar}$      $\lambda_{\text{trial}} = \frac{2m}{\hbar^2} E_0 \Rightarrow E_0 = \frac{\hbar\omega}{2}$

10/15/2021

PHY 711 Fall 2021 -- Lecture 21

8

Another example.



Recap -- Rayleigh-Ritz method of estimating the lowest eigenvalue

Example from Schroedinger equation for one-dimensional harmonic oscillator:

$$-\frac{\hbar^2}{2m} \frac{d^2 f_n(x)}{dx^2} + \frac{1}{2} m \omega^2 x^2 f_n(x) = E_n f_n(x) \quad \text{with } f_n(-\infty) = f_n(\infty) = 0$$

Trial function  $f_{\text{trial}}(x) = e^{-gx^2}$

Raleigh-Ritz estimate:  $\frac{\langle f_{\text{trial}} | S | f_{\text{trial}} \rangle}{\langle f_{\text{trial}} | \sigma | f_{\text{trial}} \rangle} = \frac{\hbar^2}{2m} \left( g + \frac{m^2 \omega^2 / \hbar^2}{4g} \right) \equiv E_{\text{trial}}(g)$

$g_0 = \frac{m\omega}{\hbar} \quad E_{\text{trial}}(g_0) = \frac{1}{2} \hbar \omega \quad \leftarrow \text{Exact answer}$

Do you think that there is a reason for getting the correct answer from this method?

- a. Chance only
- b. Skill

In this case, the minimization process yield's the exact answer.

Solution to inhomogeneous problem by using Green's functions

Inhomogeneous problem:

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

Green's function :

$$\left( -\frac{d}{dx} \tau(x) \frac{d}{dx} + v(x) - \lambda \sigma(x) \right) G_\lambda(x, x') = \delta(x - x')$$

Formal solution:

$$\varphi_\lambda(x) = \varphi_{\lambda 0}(x) + \int_a^b G_\lambda(x, x') F(x') dx'$$

Solution to homogeneous problem

10/15/2021

PHY 711 Fall 2021 – Lecture 21

10

From a knowledge of the Green's function we can find solutions of related inhomogeneous equations.

Formal solution:

$$\varphi_{\lambda}(x) = \varphi_{\lambda 0}(x) + \int_a^b G_{\lambda}(x, x') F(x') dx'$$

↙ Solution to homogeneous problem

Your question -- On slide 17, what is the homogeneous equation  $\psi_0(x)$ ?

Homogenous problem:

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

In this lecture, we will discuss several methods of finding this Green's function. This topic will also appear in PHY 712

Your question -- How do we arrive at the formal solution on slide 11?

Formal solution:

$$\varphi_{\lambda}(x) = \varphi_{\lambda_0}(x) + \int_a^b G_{\lambda}(x, x') F(x') dx'$$

Note that this form satisfies the inhomogenous equation

$$\text{Define } S(x) \equiv -\frac{d}{dx} \tau(x) \frac{d}{dx} + v(x) - \lambda \sigma(x)$$

$$S(x)\varphi_{\lambda}(x) = S(x)\varphi_{\lambda_0}(x) + S(x) \int_a^b G(x, x') F(x') dx'$$

$$S(x)\varphi_{\lambda}(x) = 0 + \int_a^b \delta(x - x') F(x') dx' = F(x)$$

Suppose that we can find a Green's function defined as follows:

$$\left( -\frac{d}{dx} \tau(x) \frac{d}{dx} + v(x) - \lambda \sigma(x) \right) G_\lambda(x, x') = \delta(x - x')$$

Recall: Completeness of eigenfunctions:

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

In terms of eigenfunctions:

$$\left( -\frac{d}{dx} \tau(x) \frac{d}{dx} + v(x) - \lambda \sigma(x) \right) G_\lambda(x, x') = \sigma(x) \sum_n \frac{f_n(x) f_n(x')}{N_n}$$

$$\Rightarrow G_\lambda(x, x') = \sum_n \frac{f_n(x) f_n(x') / N_n}{\lambda_n - \lambda} \quad \text{By construction}$$

10/15/2021

PHY 711 Fall 2021 – Lecture 21

13

The following slides present solution methods for differential equations involving the use of eigenvalues.

Example Sturm-Liouville problem:

Example:  $\tau(x) = 1$ ;  $\sigma(x) = 1$ ;  $v(x) = 0$ ;  $a = 0$  and  $b = L$

$$\lambda = 1; \quad F(x) = F_0 \sin\left(\frac{\pi x}{L}\right)$$

Inhomogenous equation:

$$\left(-\frac{d^2}{dx^2} - 1\right)\varphi(x) = F_0 \sin\left(\frac{\pi x}{L}\right)$$

Example.

Eigenvalue equation :

$$\left(-\frac{d^2}{dx^2}\right)f_n(x) = \lambda_n f_n(x)$$

Eigenfunctions

$$f_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$$

Eigenvalues :

$$\lambda_n = \left(\frac{n\pi}{L}\right)^2$$

Completeness of eigenfunctions :

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

In this example:  $\frac{2}{L} \sum_n \sin\left(\frac{n\pi x}{L}\right) \sin\left(\frac{n\pi x'}{L}\right) = \delta(x-x')$

10/15/2021

PHY 711 Fall 2021 – Lecture 21

15

Solution using eigenfunctions appropriate for this example.

Green's function :

$$\left( -\frac{d}{dx} \tau(x) \frac{d}{dx} + v(x) - \lambda \sigma(x) \right) G_\lambda(x, x') = \delta(x - x')$$

Green's function for the example :

$$G(x, x') = \sum_n \frac{f_n(x) f_n(x') / N_n}{\lambda_n - \lambda} = \frac{2}{L} \sum_n \frac{\sin\left(\frac{n\pi x}{L}\right) \sin\left(\frac{n\pi x'}{L}\right)}{\left(\frac{n\pi}{L}\right)^2 - 1}$$

Continued.



Using Green's function to solve inhomogenous equation:

$$\left(-\frac{d^2}{dx^2} - 1\right)\varphi(x) = F_0 \sin\left(\frac{\pi x}{L}\right) \quad \text{with boundary values } \varphi(0)=\varphi(L)=0$$

$$\varphi(x) = \varphi_0(x) + \int_0^L G(x, x') F_0 \sin\left(\frac{\pi x'}{L}\right) dx'$$

$$= \varphi_0(x) + \frac{2}{L} \sum_n \left[ \frac{\sin\left(\frac{n\pi x}{L}\right)}{\left(\frac{n\pi}{L}\right)^2 - 1} \int_0^L \sin\left(\frac{n\pi x'}{L}\right) F_0 \sin\left(\frac{\pi x'}{L}\right) dx' \right]$$

$$= \varphi_0(x) + \frac{F_0}{\left(\frac{\pi}{L}\right)^2 - 1} \sin\left(\frac{\pi x}{L}\right)$$

10/15/2021

PHY 711 Fall 2021 -- Lecture 21

17

In this case, the solution simplifies.

Alternate Green's function method not based on eigenvalues  
but on solutions to the homogeneous problem:

$$G(x, x') = \frac{1}{W} g_a(x_<) g_b(x_>) \quad \text{for } 0 \leq x \leq L$$

$$\left( -\frac{d^2}{dx^2} - 1 \right) g_i(x) = 0 \quad \Rightarrow g_a(x) = \sin(x); \quad g_b(x) = \sin(L-x);$$

$$W = g_b(x) \frac{dg_a(x)}{dx} - g_a(x) \frac{dg_b(x)}{dx} = \sin(L-x) \cos(x) + \sin(x) \cos(L-x) \\ = \sin(L)$$

$$\varphi(x) = \varphi_0(x) + \frac{\sin(L-x)}{\sin(L)} \int_0^x \sin(x') F_0 \sin\left(\frac{\pi x'}{L}\right) dx' \\ + \frac{\sin(x)}{\sin(L)} \int_x^L \sin(L-x') F_0 \sin\left(\frac{\pi x'}{L}\right) dx'$$

$$\varphi(x) = \varphi_0(x) + \frac{F_0}{\left(\frac{\pi}{L}\right)^2 - 1} \sin\left(\frac{\pi x}{L}\right) \quad \text{(Actually the algebra is painful).}$$

But, hurray! Same result as before.

10/15/2021

PHY 711 Fall 2021 – Lecture 21

18

Another method of finding a Green's function.

More details on the general method of constructing Green's functions using homogeneous solution

Green's function :

$$\left( -\frac{d}{dx} \tau(x) \frac{d}{dx} + v(x) - \lambda \sigma(x) \right) G_\lambda(x, x') = \delta(x - x')$$

Two homogeneous solutions

$$\left( -\frac{d}{dx} \tau(x) \frac{d}{dx} + v(x) - \lambda \sigma(x) \right) g_i(x) = 0 \quad \text{for } i = a, b$$

Let

$$G_\lambda(x, x') = \frac{1}{W} g_a(x_<) g_b(x_>)$$

10/15/2021

PHY 711 Fall 2021 -- Lecture 21

19

Green's function based on homogeneous solutions (not eigenfunctions).

For  $\epsilon \rightarrow 0$ :

$$\int_{x'-\epsilon}^{x'+\epsilon} dx \left( -\frac{d}{dx} \tau(x) \frac{d}{dx} + v(x) - \lambda \sigma(x) \right) G_\lambda(x, x') = \int_{x'-\epsilon}^{x'+\epsilon} dx \delta(x - x')$$

$$\int_{x'-\epsilon}^{x'+\epsilon} dx \left( -\frac{d}{dx} \tau(x) \frac{d}{dx} \right) \frac{1}{W} g_a(x_<) g_b(x_>) = 1$$

$$-\frac{\tau(x)}{W} \left( \frac{d}{dx} g_a(x_<) g_b(x_>) \right) \Big|_{x'-\epsilon}^{x'+\epsilon} = \frac{\tau(x')}{W} \left( g_a(x') \frac{d}{dx} g_b(x') - g_b(x') \frac{d}{dx} g_a(x') \right)$$

$$\Rightarrow W = \tau(x') \left( g_a(x') \frac{d}{dx} g_b(x') - g_b(x') \frac{d}{dx} g_a(x') \right)$$

Note --  $W$  (Wronskian) is constant, since  $\frac{dW}{dx'} = 0$ .

$\Rightarrow$  Useful Green's function construction in one dimension:

$$G_\lambda(x, x') = \frac{1}{W} g_a(x_<) g_b(x_>)$$

10/15/2021

PHY 711 Fall 2021 -- Lecture 21

20

Some details.

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

Green's function solution:

$$\begin{aligned} \varphi_{\lambda}(x) &= \varphi_{\lambda 0}(x) + \int_a^b G_{\lambda}(x, x') F(x') dx' \\ &= \varphi_{\lambda 0}(x) + \frac{g_b(x)}{W} \int_a^x g_a(x') F(x') dx' + \frac{g_a(x)}{W} \int_x^b g_b(x') F(x') dx' \end{aligned}$$

Note that the integral has to be performed in two parts. While the eigenfunction expansion method can be generalized to 2 and 3 dimensions, this method only works for one dimension.

More details.

Another example --

$$\frac{d^2}{dx^2} \Phi(x) = -\rho(x) / \epsilon_0 \quad \text{electrostatic potential for charge density } \rho(x)$$

Homogeneous equation:

$$\frac{d^2}{dx^2} g_{a,b}(x) = 0$$

$$\text{Let } g_a(x) = x \quad g_b(x) = 1$$

Wronskian:

$$W = g_a(x) \frac{dg_b(x)}{dx} - g_b(x) \frac{dg_a(x)}{dx} = -1$$

Green's function:

$$G(x, x') = -x_{<}$$

$$\Phi(x) = \Phi_0(x) + \frac{1}{\epsilon_0} \int_{-\infty}^x dx' x' \rho(x') + \frac{x}{\epsilon_0} \int_x^{\infty} dx' \rho(x')$$

10/15/2021

PHY 711 Fall 2021 -- Lecture 21

22

Another example, this time taken from electrostatics.

Example -- continued

$$\frac{d^2}{dx^2} \Phi(x) = -\rho(x) / \epsilon_0 \quad \text{electrostatic potential for charge density } \rho(x)$$

$$\Phi(x) = \Phi_0(x) + \frac{1}{\epsilon_0} \int_{-\infty}^x dx' x' \rho(x') + \frac{x}{\epsilon_0} \int_x^{\infty} dx' \rho(x')$$

$$\text{Suppose } \rho(x) = \begin{cases} 0 & x \leq -a \\ \rho_0 x / a & -a \leq x \leq a \\ 0 & x \geq a \end{cases}$$

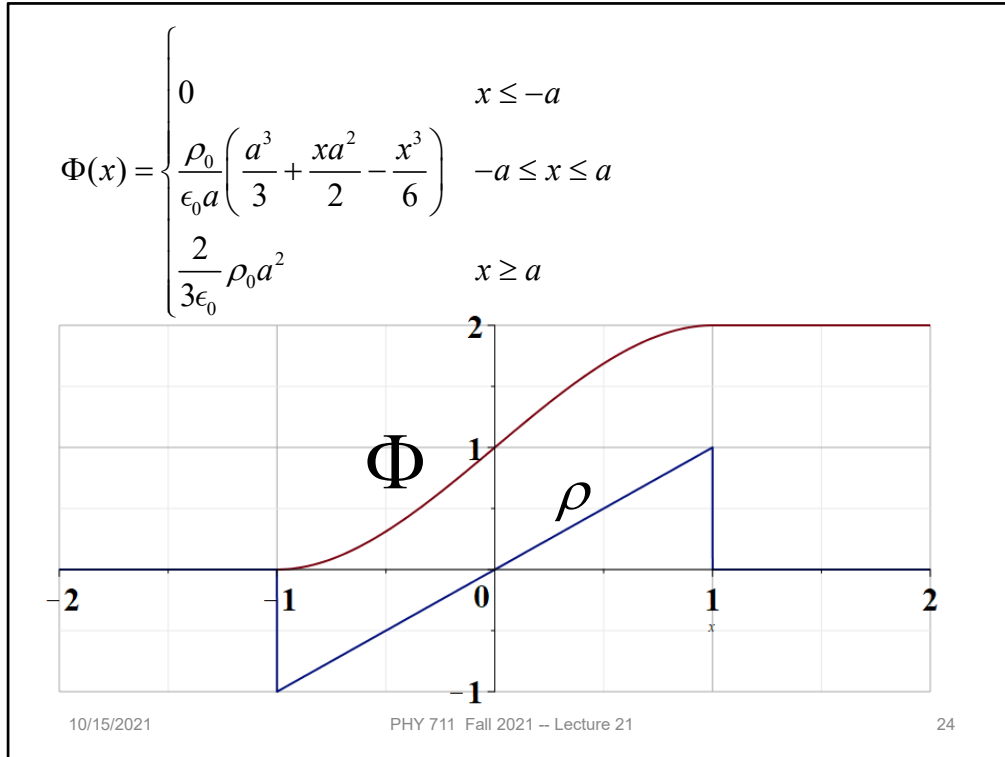
$$\Phi(x) = \Phi_0(x) + \begin{cases} 0 & x \leq -a \\ \frac{\rho_0}{\epsilon_0 a} \left( \frac{a^3}{3} + \frac{xa^2}{2} - \frac{x^3}{6} \right) & -a \leq x \leq a \\ \frac{2}{3\epsilon_0} \rho_0 a^2 & x \geq a \end{cases}$$

10/15/2021

PHY 711 Fall 2021 -- Lecture 21

23

Solutions for a particular charge distribution.



Plot of the charge distribution and of the electrostatic potential.