

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

Plan for Lecture 17:

Continue reading Chapter 7

1. The wave equation
2. Sturm-Liouville equation
3. Green's function solution methods

10/2/2019 PHY 711 Fall 2019 – Lecture 17 1

1

Wake Forest College & Graduate School of Arts and Sciences

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WFU Physics People Events and News Undergraduate Graduate Research Resources f g t s

Events

Colloquium: "Modeling of Excited State Dynamics in Confined and Periodic Nanostructures" – Wednesday Oct. 2, 2019 at 3 PM
 Professor Dmitri Klin Department of Chemistry and Biochemistry North Dakota State University Fargo, ND George P. Williams, Jr. Lecture Hall (Olin 101) Wednesday, Oct. 2, 2019 at 3:00 PM There ...

Colloquium: "Mechanism of H-atom Atom-Surface Scattering Arrangement Catalyzed by Radial SAM Enclosures" – Wednesday Oct. 9, 2019 at 3 PM
 Professor Troy Stich Department of Chemistry Wake Forest University George P. Williams, Jr. Lecture Hall (Olin 101) Wednesday, Oct. 9, 2019, at 3:00 PM There will be a reception in ...

10/2/2019 PHY 711 Fall 2019 – Lecture 17 2

2



Date	F&W Reading	Topic	Assignment	Due
1 Mon, 8/26/2019	Chap. 1	Introduction	#1	8/30/2019
2 Wed, 8/28/2019	Chap. 1	Scattering theory	#2	9/02/2019
3 Fri, 8/30/2019	Chap. 1	Scattering theory	#3	9/04/2019
4 Mon, 9/02/2019	Chap. 1	Scattering theory	#4	9/06/2019
5 Wed, 9/04/2019	Chap. 2	Non-inertial coordinate systems	#5	9/09/2019
6 Fri, 9/06/2019	Chap. 3	Calculus of Variation	#6	9/11/2019
7 Mon, 9/9/2019	Chap. 3	Calculus of Variation	#7	9/13/2019
8 Wed, 9/11/2019	Chap. 3	Lagrangian Mechanics		
9 Fri, 9/13/2019	Chap. 3	Lagrangian Mechanics	#8	9/16/2019
10 Mon, 9/16/2019	Chap. 3 & 6	Constants of the motion	#9	9/20/2019
11 Wed, 9/18/2019	Chap. 3 & 6	Hamiltonian equations of motion		
12 Fri, 9/20/2019	Chap. 3 & 6	Liouville theorem	#10	9/23/2019
13 Mon, 9/23/2019	Chap. 3 & 6	Canonical transformations		
14 Wed, 9/25/2019	Chap. 4	Small oscillations about equilibrium	#11	9/30/2019
15 Fri, 9/27/2019	Chap. 4	Normal modes of vibration	#12	10/02/2019
16 Mon, 9/30/2019	Chap. 7	Motion of strings	#13	10/04/2019
17 Wed, 10/02/2019	Chap. 7	Sturm-Liouville equations	#14	10/07/2019
18 Fri, 10/04/2019	Chap. 7	Sturm-Liouville equations		
19 Mon, 10/07/2019	Chap. 7	Fourier transform methods		
20 Wed, 10/09/2019	Chap. 1-4,6-7	Review		
Fri, 10/11/2019	No class	Fall break		
Mon, 10/14/2019	No class	Take-home exam		
Wed, 10/16/2019	No class	Take-home exam		
21 Fri, 10/18/2019	Chap. 7	Take-home exam due		

10/2/2019 PHY 711 Fall 2019 – Lecture 17 3

3

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

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.

10/2/2019

PHY 711 Fall 2019 – Lecture 17

4

4

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 spacially 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:

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

Sturm-Liouville equation for spatial function:

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

10/2/2019

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5

5

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 solution to be determined applied force

Homogenous problem: $F(x)=0$

10/2/2019

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6

6

Examples of Sturm-Liouville eigenvalue equations --

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

Bessel functions:

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

Legendre functions:

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

Fourier functions:

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

10/2/2019

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7

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:

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

10/2/2019

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8

Comment on orthogonality of eigenfunctions

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

10/2/2019

PHY 711 Fall 2019 – Lecture 17

9

9

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 $a \leq x \leq b$:

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


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

10/2/2019 PHY 711 Fall 2019 – Lecture 17 10

10

Comment on orthogonality of eigenfunctions -- continued

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

Possible boundary values for Sturm-Liouville equations:

1. $f_m(a) = f_m(b) = 0$
2. $\tau(x) \frac{df_m(x)}{dx} \Big|_a^b = \tau(x) \frac{df_m(x)}{dx} \Big|_b = 0$
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:

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

10/2/2019 PHY 711 Fall 2019 – Lecture 17 11

11

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:

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

10/2/2019 PHY 711 Fall 2019 – Lecture 17 12

12

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:

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

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

10/2/2019

PHY 711 Fall 2019 – Lecture 17

13

13

Variation approximation to lowest eigenvalue

In general, there are several techniques to determine the eigenvalues λ_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

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

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.

10/2/2019

PHY 711 Fall 2019 – Lecture 17

14

14

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:

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

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

10/2/2019

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15

15

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

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

10/2/2019

PHY 711 Fall 2019 – Lecture 17

16

16

Green's function solution methods

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

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

Completeness of eigenfunctions:

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

In terms of eigenfunctions:

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

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

10/2/2019

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17

17

Solution to inhomogeneous problem by using Green's functions

Inhomogenous problem:

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

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:

$$\phi_\lambda(x) = \phi_{\lambda 0}(x) + \int_0^L G_\lambda(x, x') F(x') dx'$$

Solution to homogeneous problem

10/2/2019

PHY 711 Fall 2019 – Lecture 17

18

18

Example Sturm-Liouville problem:

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

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

Inhomogenous equation :

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

10/2/2019

PHY 711 Fall 2019 -- Lecture 17

19

19

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

10/2/2019

PHY 711 Fall 2019 -- Lecture 17

20

20

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 :

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

10/2/2019

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21

21

Using Green's function to solve inhomogeneous equation :

$$\begin{aligned} \left(-\frac{d^2}{dx^2} - 1 \right) \phi(x) &= F_0 \sin\left(\frac{\pi x}{L}\right) \\ \phi(x) &= \phi_0(x) + \int_0^L G(x, x') F_0 \sin\left(\frac{\pi x'}{L}\right) dx' \\ &= \phi_0(x) + \frac{2}{L} \sum_n \left[\frac{\sin\left(\frac{n\pi x}{L}\right)}{\left(\frac{n\pi}{L}\right)^2 - 1} \int_0^L \sin\left(\frac{n\pi x'}{L}\right) F_0 \sin\left(\frac{\pi x'}{L}\right) dx' \right] \\ &= \phi_0(x) + \frac{F_0}{\left(\frac{\pi}{L}\right)^2 - 1} \sin\left(\frac{\pi x}{L}\right) \end{aligned}$$

10/2/2019

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22

22

Alternate Green's function method:

$$\begin{aligned} G(x, x') &= \frac{1}{W} g_a(x_{<}) g_b(x_{>}) \\ \left(-\frac{d^2}{dx^2} - 1 \right) g_i(x) &= 0 \quad \Rightarrow g_a(x) = \sin(x); \quad g_b(x) = \sin(L-x); \\ W &= g_b(x) \frac{dg_a(x)}{dx} - g_a(x) \frac{dg_b(x)}{dx} = \sin(L-x) \cos(x) + \sin(x) \cos(L-x) \\ &= \sin(L) \\ \phi(x) &= \phi_0(x) + \frac{\sin(L-x)}{\sin(L)} \int_0^x \sin(x') F_0 \sin\left(\frac{\pi x'}{L}\right) dx' \\ &\quad + \frac{\sin(x)}{\sin(L)} \int_x^L \sin(L-x') F_0 \sin\left(\frac{\pi x'}{L}\right) dx' \\ \phi(x) &= \phi_0(x) + \frac{F_0}{\left(\frac{\pi}{L}\right)^2 - 1} \sin\left(\frac{\pi x}{L}\right) \end{aligned}$$

10/2/2019

PHY 711 Fall 2019 -- Lecture 17

23

23

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

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

10/2/2019

PHY 711 Fall 2019 -- Lecture 17

24

24

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:

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

10/2/2019

PHY 711 Fall 2019 – Lecture 17

25

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

Green's function solution:

$$\begin{aligned} \phi_\lambda(x) &= \phi_{\lambda 0}(x) + \int_{x_l}^{x_u} G_\lambda(x, x') F(x') dx' \\ &= \phi_{\lambda 0}(x) + \frac{g_b(x)}{W} \int_{x_l}^x g_a(x') F(x') dx' + \frac{g_a(x)}{W} \int_x^{x_u} g_b(x') F(x') dx' \end{aligned}$$

10/2/2019

PHY 711 Fall 2019 – Lecture 17

26

26