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

Notes on Lecture 22 – 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

19	Mon, 10/03/2022	Chap. 7	Sturm-Liouville equations	#15	10/05/2022
20	Wed, 10/05/2022	Chap. 7	Sturm-Liouville equations		
21	Fri, 10/07/2022	Chap. 1-4,6-7	Review		
	Mon, 10/10/2022	No class	Take home exam		
	Wed, 10/12/2022	No class	Take home exam		
	Fri, 10/14/2022	No class	Fall break		
22	Mon, 10/17/2022	Chap. 7	Green's function methods for one-dimensional Sturm-Liouville equations	#16	10/19/2022
23	Wed, 10/19/2022	Chap. 7	Fourier and other transform methods		

PHY 711 -- Assignment #16

Oct. 17, 2022

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

Consider the example presented in the last two slides of Lecture 22, where a one-dimensional Poisson equation was solved using a Green's function constructed from the corresponding homogeneous solutions. Verify the results on this slide and check that the resultant potential $\Phi(x)$ satisfies the particular Poisson equation for $x \leq -a$, $-a \leq x \leq a$, and for $x \geq a$.

Your questions –

From Sam -- I am still not quite understanding how the Rayleigh Ritz method works. It seems that after the cancellations of the expectation values on top and bottom, you should be left with the sum of lambda n over all n, and while that is greater than lambda 0, I don't get how it approximates it.

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

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

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.

Eigenvalues and eigenfunctions of Sturm-Liouville equations

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

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

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 λ_n are real

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

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

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

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

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 $f_n(x)$:

$\tilde{h}(x) = \sum_n C_n f_n(x),$ where the coefficients C_n can be assumed to be real.

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:

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

It also follows that:

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

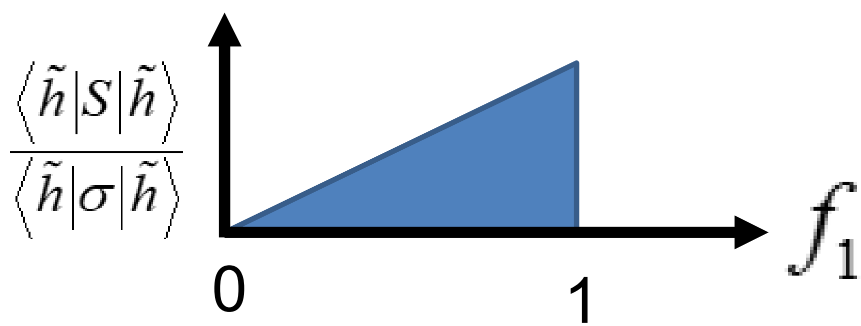
Therefore $$\frac{\left\langle \tilde{h} \middle| S \middle| \tilde{h} \right\rangle}{\left\langle \tilde{h} \middle| \sigma \middle| \tilde{h} \right\rangle} = \frac{\sum_n |C_n|^2 N_n \lambda_n}{\sum_n |C_n|^2 N_n} \geq \lambda_0.$$

Some additional comments -- $\dfrac{\langle \tilde{h}|S|\tilde{h}\rangle}{\langle \tilde{h}|\sigma|\tilde{h}\rangle} = \dfrac{\sum_n |C_n|^2 N_n \lambda_n}{\sum_n |C_n|^2 N_n} \geq \lambda_0.$

$$\frac{\langle \tilde{h}|S|\tilde{h}\rangle}{\langle \tilde{h}|\sigma|\tilde{h}\rangle} = \sum_{n=0}^{\infty} f_n \lambda_n \qquad \text{where} \quad \sum_{n=0}^{\infty} f_n = 1$$

For the case of only two non-trivial eigenvalues:

$$\frac{\langle \tilde{h}|S|\tilde{h}\rangle}{\langle \tilde{h}|\sigma|\tilde{h}\rangle} = f_0\lambda_0 + f_1\lambda_1 = \lambda_0 + (\lambda_1 - \lambda_0) f_1$$



Rayleigh-Ritz method of estimating the lowest eigenvalue

$$\lambda_0 \le \frac{\left\langle \tilde{h} \middle| S \middle| \tilde{h} \right\rangle}{\left\langle \tilde{h} \middle| \sigma \middle| \tilde{h} \right\rangle},$$

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

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

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

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

Rayleigh-Ritz method of estimating the lowest eigenvalue

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

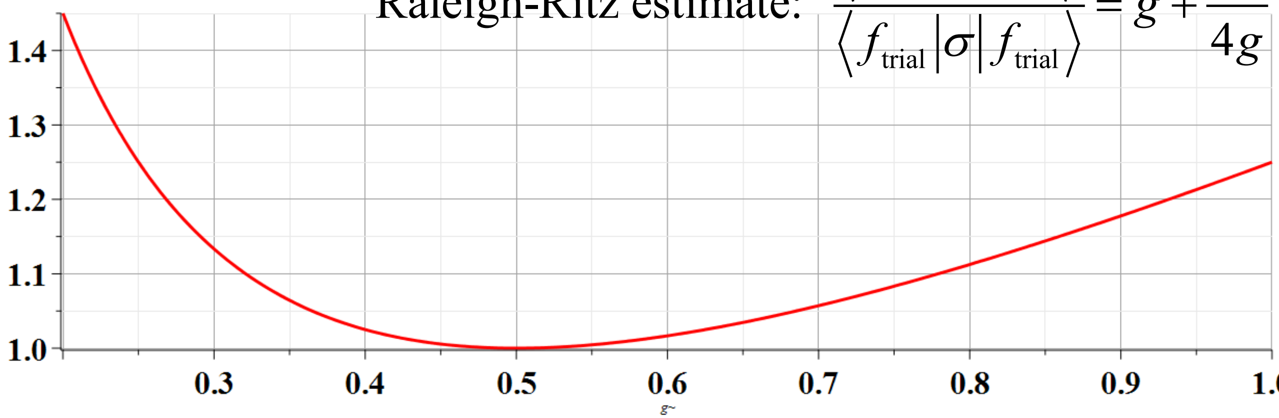
Another example – this time with a variable parameter

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

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

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

$$\frac{\lambda_{\text{trial}}(g)}{\sqrt{G}}$$



$$g / \sqrt{G}$$

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

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

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

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

Example from Schroedinger equation for one-dimensional harmonic oscillator:

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

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

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

$g_0=\dfrac{m\omega}{\hbar} \qquad E_{\text{trial}}(g_0)=\dfrac{1}{2}\hbar\omega$ ⇦ Exact answer

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

a. Chance only
b. Skill

Solution to inhomogeneous problem by using Green's functions

Inhomogenous problem:

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

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

Formal solution:

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

Solution to homogeneous problem

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

How do we arrive at the formal solution?

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

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

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

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

Using complete set of eigenfunctions to form Green's function --

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

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

Recall:

Completeness of eigenfunctions:

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

In terms of eigenfunctions:

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

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

By construction

Example Sturm-Liouville problem:

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

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

Inhomogenous equation:

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

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:

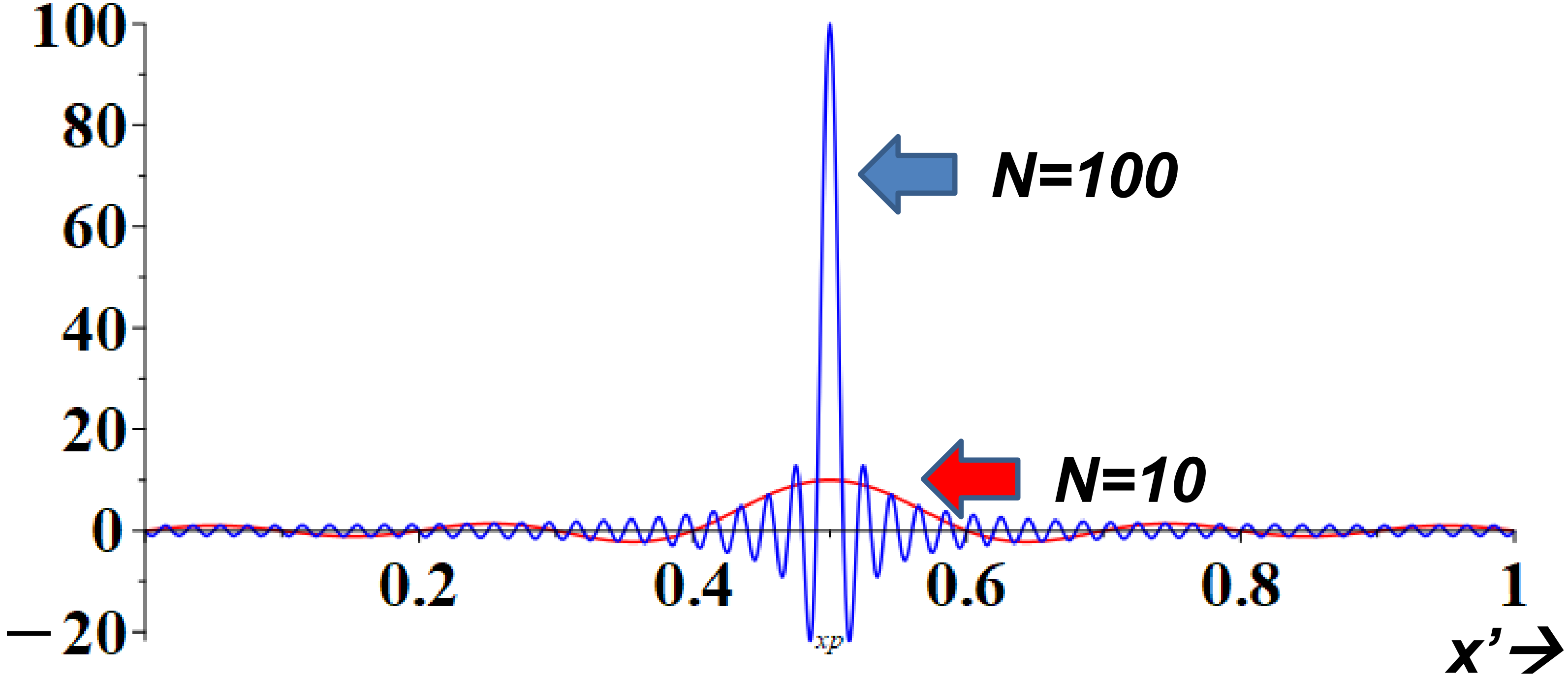
$$\sigma(x)\sum_n \frac{f_n(x)f_n(x')}{N_n}=\delta(x-x')$$

In this example:

$$\frac{2}{L}\sum_{n=1}^{\infty}\sin\left(\frac{n\pi x}{L}\right)\sin\left(\frac{n\pi x'}{L}\right)=\delta(x-x')$$

In reality, for finite summation $$\frac{2}{L}\sum_{n=1}^{N}\sin\left(\frac{n\pi x}{L}\right)\sin\left(\frac{n\pi x'}{L}\right)=\delta(x-x')$$

x=1/2, L=1



Green's function :

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

Green's function for the example :

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

Using Green's function to solve inhomogenous equation:

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

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

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

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

Another method of constructing Green's functions -- using two solutions to the homogeneous problem

Green's function:

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

Two homogeneous solutions

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

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

$$\text{where } W\equiv\tau(x')\left(g_a(x')\frac{d}{dx}g_b(x')-g_b(x')\frac{d}{dx}g_a(x')\right)$$

Some details:

For $\epsilon \to 0$:

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

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

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

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

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

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

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

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

Green's function solution:

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

$$=\varphi_{\lambda 0}(x)+\frac{g_b(x)}{W}\int_a^x g_a(x')F(x')dx'+\frac{g_a(x)}{W}\int_x^b g_b(x')F(x')dx'$$

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.

Example from previous discussion:

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

Using: $G(x,x')=\frac{1}{W}g_a(x_<)g_b(x_>)$ for $0\le x\le L$

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

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

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

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

(Actually the algebra is painful).
But, hurray! Same result as before.

Another example --

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

Homogeneous equation:

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

Let $g_a(x) = x \qquad g_b(x) = 1$

Wronskian:

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

Green's function:

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

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

Example -- continued

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

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

Suppose $\rho(x) = \begin{cases} 0 & x \le -a \\ \rho_0 x / a & -a \le x \le a \\ 0 & x \ge a \end{cases}$

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

$$\Phi(x) = \begin{cases} 0 & x \le -a \\ \dfrac{\rho_0}{\epsilon_0 a}\left(\dfrac{a^3}{3} + \dfrac{xa^2}{2} - \dfrac{x^3}{6}\right) & -a \le x \le a \\ \dfrac{2}{3\epsilon_0}\rho_0 a^2 & x \ge a \end{cases}$$