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 $x \geq a$.

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 $a \leq x \leq b$:

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

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

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

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

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

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:

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

It also follows that:

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

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

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

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

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

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

Rayleigh-Ritz method of estimating the lowest eigenvalue

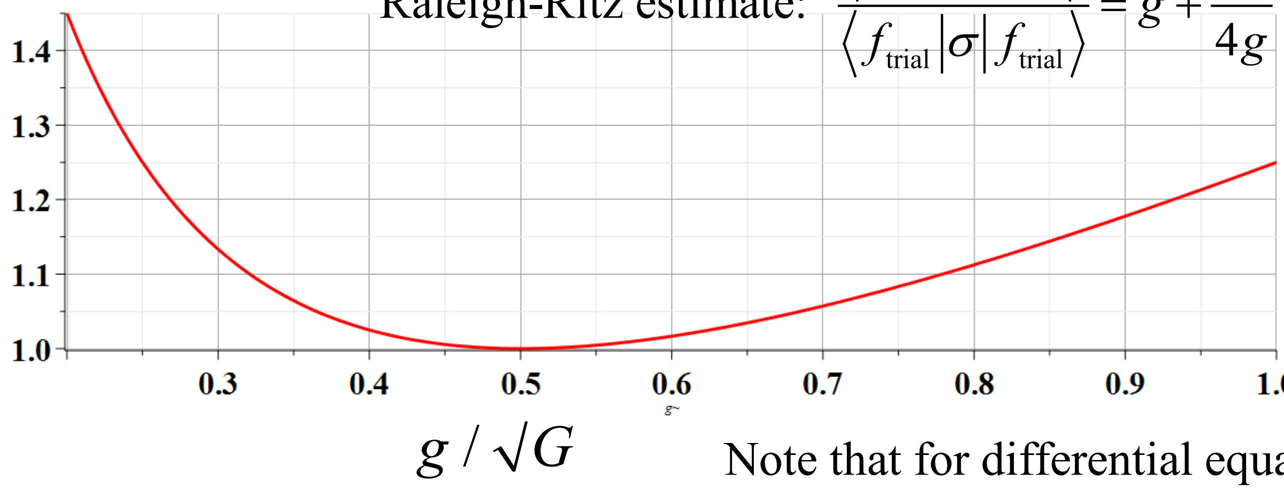
$$\lambda_0 \le \frac{\langle \tilde{h} | S | \tilde{h} \rangle}{\langle \tilde{h} | \sigma | \tilde{h} \rangle},$$

Another example – this time with a variable parameter

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

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

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



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

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

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

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

$$g_0=\frac{m\omega}{\hbar} \qquad E_{\text{trial}}(g_0)=\frac{1}{2}\hbar\omega$$

⇐ 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:

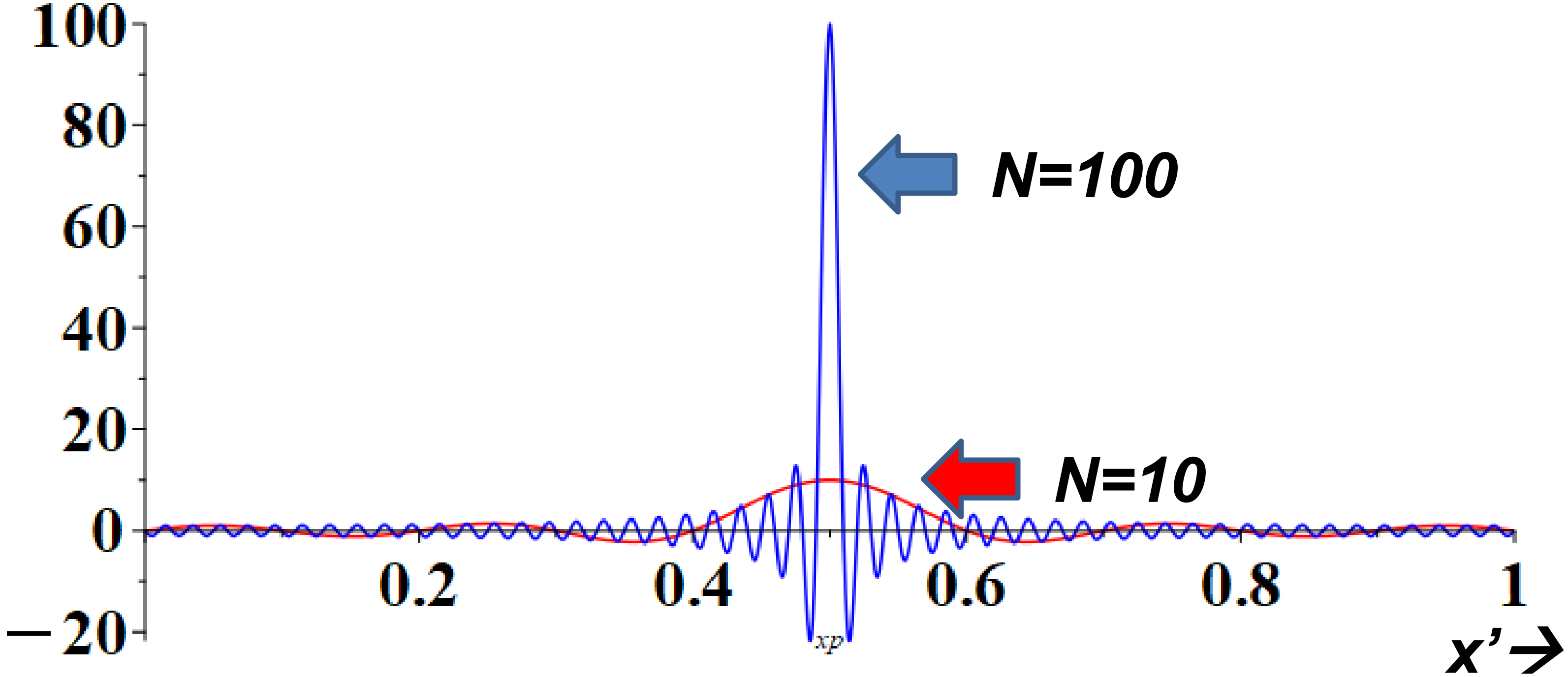
$$\sigma(x) \sum_n \frac{f_n(x) f_n(x')}{N_n} = \delta(x - x')$$

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

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

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

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 $\epsilon \rightarrow 0$:

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

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

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

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

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:

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

$$\frac{d^2}{dx^2}\Phi(x) = -\rho(x)/\epsilon_0$$ 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

$$\frac{d^2}{dx^2}\Phi(x) = -\rho(x)/\epsilon_0$$ 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 $\rho(x) = \begin{cases} 0 & x \le -a \\ \rho_0 x/a & -a \le x \le a \\ 0 & x \ge a \end{cases}$

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

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