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

Notes on Lecture 20 – Chap. 7 (F&W)

Properties of Sturm-Liouville equations

1. Eigenfunctions of Sturm-Liouville equation
2. Notion of the completeness property of eigenvalue expansions
3. Green's function solution methods

PHYSICS COLLOQUIUM

THURSDAY

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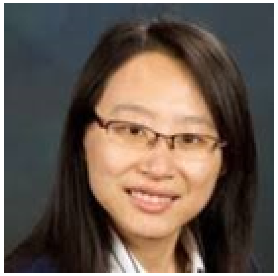
OCTOBER 6, 2022

Carrier Transport in 2D Perovskite Semiconductors and its Application in High Performance X-ray Sensing



Ruddlesden–Popper (RP) phase 2D perovskites are recent emerging materials for photovoltaics, light emitting diodes and radiation sensing. RP perovskites are nanostructured material in a naturally formed quantum well geometry, that have been integrated in functional devices, featuring with greatly extended operational lifetimes. Recently, it is found that the carrier transport properties are pretty unique in the 2D RP perovskite crystal and thin films. A luminescent "edge state" was discovered that greatly impact the carrier transport and recombination processes.

In this talk, I will first discuss the unique carrier transport properties of 2D perovskite single crystals. Using a scanning photocurrent microscopy technique, we probed an unusually long carrier diffusion length in the RP perovskite single crystals. We attributed it to the intrinsically existing shallow trap that extended the carrier lifetime via trapping/de-trapping process. Next, I will talk about the 2D RP perovskites in radiation detector applications. We integrated the quasi-2D perovskite polycrystalline film into photodiodes and achieved high X-ray

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4:00 pm - Olin 101*

*Link provided for those unable to attend in person.

Note: For additional information on the seminar or to obtain the video conference link, contact wfuphys@wfu.edu

Reception at 3:30pm - Olin Entrance

Your questions –

From Zezhong -- In your PPT, you used some Dirac notations from quantum physics as equations. Do they have the same calculation methods as quantum physics?

From Sam -- I was wondering what sort of systems could be described by these equations, or the scenarios in which you would use these methods.

15	Fri, 9/23/2022	Chap. 4	Small oscillations about equilibrium	#12	9/26/2022
16	Mon, 9/26/2022	Chap. 4	Normal modes of vibration	#13	9/28/2022
17	Wed, 9/28/2022	Chap. 4	Normal modes of more complicated systems	#14	10/03/2022
18	Fri, 9/30/2022	Chap. 7	Motion of strings		
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	Class resumes		

The wave equation and related linear PDE's

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

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

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:

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

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: $0 \le x \le \infty$

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

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

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

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

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

Solution methods of Sturm-Liouville equations (assume all functions and constants are real):

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

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

Eigenfunctions:

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

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

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

Completeness of eigenfunctions:

This leads to: ➔

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

Comment on orthogonality of eigenfunctions

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

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

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

$$=\left(\lambda_n-\lambda_m\right)\sigma(x)f_n(x)f_m(x)$$

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

Comment on orthogonality of eigenfunctions -- continued

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

Now consider integrating both sides of the equation in the interval

$a \leq x \leq b$:

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

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

Comment on orthogonality of eigenfunctions -- continued

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

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 $f_n(x)$

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

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

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

For an arbitrary function: $$h(x) \approx \sum_n C_n f_n(x),$$

where $$C_n = \frac{1}{N_n}\int_a^b \sigma(x')h(x')f_n(x')dx' \quad \text{with} \quad N_n = \int_a^b \sigma(x')\left(f_n(x')\right)^2$$

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:

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

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

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

$$\Rightarrow h(x) = \sum_n \left(\left(\frac{1}{N_n}\int_a^b \sigma(x')h(x')f_n(x')dx' \right) f_n(x) \right)$$

We also know that for $a \le x \le b$, $h(x) = \int_a^b \delta(x-x')h(x')$

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

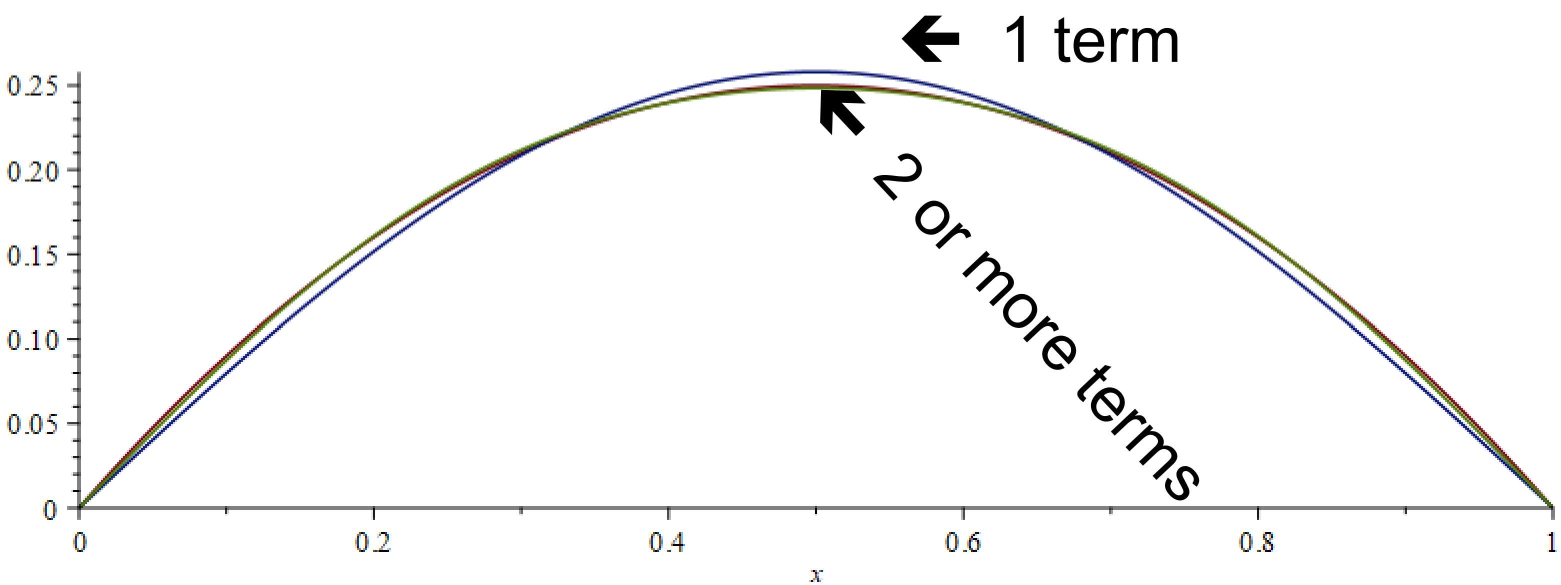
This is the completeness property of the eigenfunctions. How many terms are needed for the expansion, depends on both the function *h(x)* and on the eigenfunctions $f_n(x)$.

Example: Suppose $0 \le x \le 1$ and $-\dfrac{d^2 f_n(x)}{dx^2} = n^2\pi^2 f_n(x)$

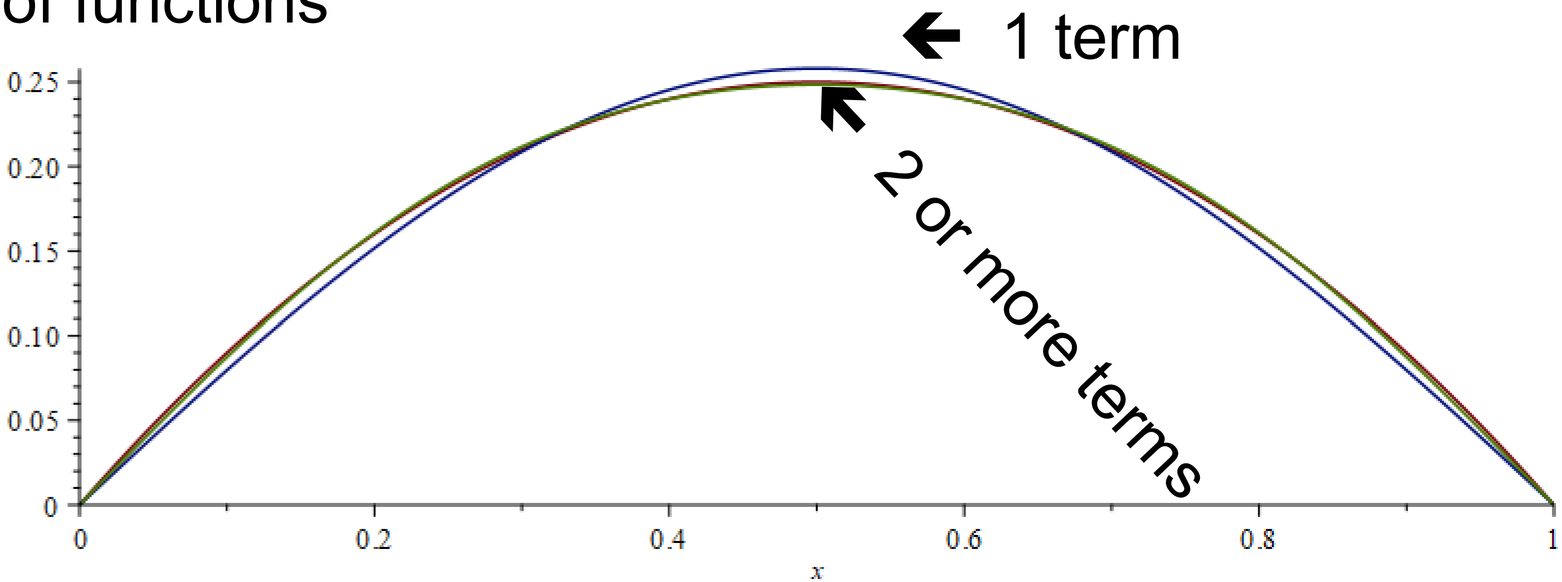
$$f_n(x) = sin(n\pi x) \qquad N_n = \frac{1}{2}$$

Now consider $h(x) = x(1-x)$

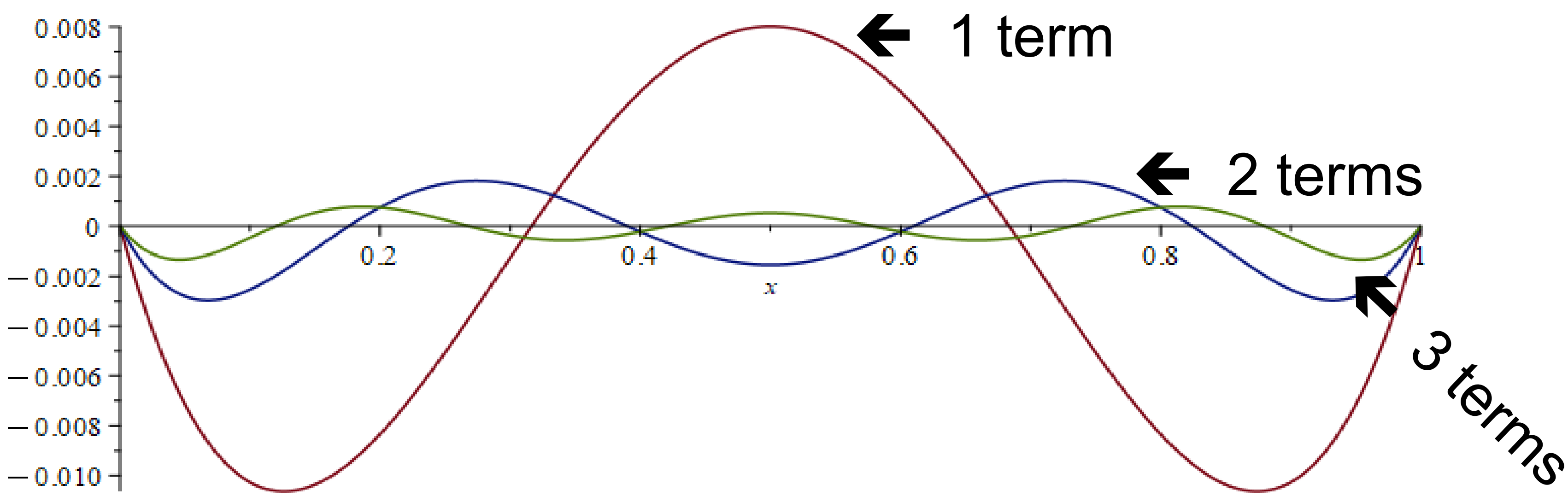
$$\mathrm{C}_n = 2\int_0^1 h(x')sin(n\pi x')dx' = \begin{cases} \dfrac{8}{n^3\pi^3} & \text{for n odd} \\ 0 & \text{for n even} \end{cases}$$



Plot of functions



Plot of error in expansion



Variational 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

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

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

Where λ_0 denotes the lowest eigenvalue.

Rayleigh-Ritz method of estimating the lowest eigenvalue

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

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

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

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

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

Another example – this time from Quantum Mechanics

Variational method for estimating ground state energy of a H atom:

Define $f(\psi) \equiv \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle}$ $\qquad \min_\psi f(\psi) \geq E_0$

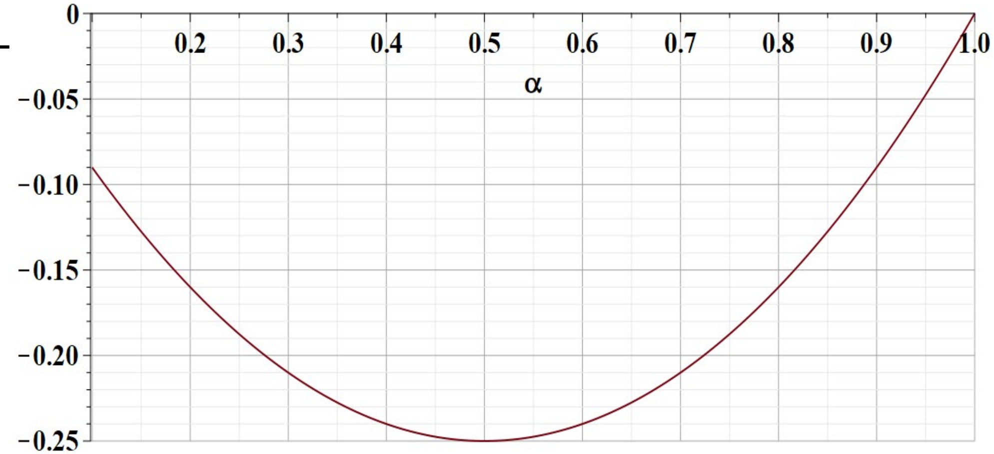
Example: $H(\mathbf{r}) = -\frac{\hbar^2}{2\mu}\nabla_r^2 - \frac{Ze^2}{r}$

Try: $|\psi\rangle = e^{-\alpha r}$

$$f(\psi) = \frac{\hbar^2}{2\mu}\alpha^2 - Ze^2\alpha$$

$$\frac{df}{d\alpha} = 0 \qquad \Rightarrow \alpha = \frac{Ze^2\mu}{\hbar^2} = \frac{Z}{a_0} \qquad \Rightarrow \min_\psi f(\psi) = -\frac{Z^2e^2}{2a_0}$$

Example: $H(\mathbf{r}) = -\frac{\hbar^2}{2\mu}\nabla_r^2 - \frac{Ze^2}{r}$



Try: $|\psi\rangle = e^{-\alpha r}$

$$f(\psi) = \frac{\hbar^2}{2\mu}\alpha^2 - Ze^2\alpha$$

$$\left.\frac{df}{d\alpha}\right|_{\alpha_{opt}} = 0 \qquad \Rightarrow \alpha_{opt} = \frac{Ze^2\mu}{\hbar^2} = \frac{Z}{a_0}$$

α_{opt}

$$\boxed{\Rightarrow \min_{\psi} f(\psi) = -\frac{Z^2e^2}{2a_0}}$$

Does this look familiar?

Variational methods for estimating ground state energy

-- continued

Example: $H(\mathbf{r}) = -\frac{\hbar^2}{2\mu}\nabla_r^2 - \frac{Ze^2}{r}$

Try: $|\psi\rangle = e^{-\alpha r^2}$

A different trial wavefunction choice.

$$f(\psi) = \frac{\hbar^2}{2\mu}6\alpha - \frac{4Ze^2\sqrt{\alpha}}{\sqrt{\pi}}$$

$$\frac{df}{d\alpha} = 0 \qquad \Rightarrow \alpha = \frac{4Z^2}{9a_0^2\pi}$$

$$\min_\psi f(\psi) = -\frac{Z^2e^2}{2a_0}\frac{8}{3\pi}$$

How do you interpret this result?

A generally useful solution method -- Green's function approach

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:

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

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

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:

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

Solution to homogeneous problem

Example Sturm-Liouville problem:

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

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

Inhomogenous equation :

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

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

Green's function :

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

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 :

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

$$\phi(x) = \phi_0(x) + \int_0^L G(x,x')F_0 \sin\left(\frac{\pi x'}{L}\right)dx'$$

$$= \phi_0(x) + \frac{2}{L}\sum_n \left[\frac{\sin\left(\frac{n\pi x}{L}\right)}{\left(\frac{n\pi}{L}\right)^2-1}\int_0^L \sin\left(\frac{n\pi x'}{L}\right)F_0 \sin\left(\frac{\pi x'}{L}\right)dx'\right]$$

$$= \phi_0(x) + \frac{F_0}{\left(\frac{\pi}{L}\right)^2-1}\sin\left(\frac{\pi x}{L}\right)$$

Alternate Green's function method:

These slides were not covered in class.

$$G(x,x')=\frac{1}{W}g_a(x_<)g_B(x_>)$$

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

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

$$=\ \sin(L)$$

$$\phi(x)=\phi_0(x)+\frac{\sin(L-x)}{\sin(L)}\int_0^x \sin(x')F_0\sin\left(\frac{\pi x'}{L}\right)dx'$$

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

$$\phi(x)=\phi_0(x)+\frac{F_0}{\left(\frac{\pi}{L}\right)^2-1}\sin\left(\frac{\pi x}{L}\right)$$

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

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

Let

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

For $\epsilon \to 0$:

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

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

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

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

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

$\Rightarrow$ 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:

$$\varphi_\lambda(x)=\varphi_{\lambda 0}(x)+\int_{x_l}^{x_u}G_\lambda(x,x')F(x')dx'$$

$$=\varphi_{\lambda 0}(x)+\frac{g_b(x)}{W}\int_{x_l}^{x}g_a(x')F(x')dx'+\frac{g_a(x)}{W}\int_{x}^{x_u}g_b(x')F(x')dx'$$