Sturm-Liouville equation

Last time, when studying the problem with a convective boundary condition, after using separation of variables for the transient solution we arrived at the eigenequation:

$$\frac{d^2X}{dx^2} = -k^2 X(x) \tag{1}$$

with BC $X(0) = 0$, $\frac{dX}{dx}|_{x=a} = \beta X(a)$. This lead to the eigenfunctions

$$X_n(x) = \sin(k_n x)$$

corresponding to the eigenvalues k_n, $n = 1, 2, ...$, which are the solutions of the equation

$$\beta \tan(k_n a) = k_n.$$

I stated that these eigenfunctions have the property that if

$$k_n \neq k_m \to \int_0^a dx X_n(x) X_m(x) = 0. \tag{2}$$

This is extremely useful because it allows us to find the coefficients in a general expansion, namely if for any $x \in [0, a]$:

$$f(x) = \sum_{n=1}^{\infty} a_n X_n(x) \to \int_0^a dx f(x) X_m(x) = a_m \int_0^a dx [X_m(x)]^2$$

since all other terms in the sum vanish. Therefore, :

$$a_m = \frac{\int_0^a dx f(x) X_m(x)}{\int_0^a dx [X_m(x)]^2}, (\forall) m = 1, 2, ...$$

and the problem is solved.

It turns out that Eq. (2), i.e. the fact that **eigenfunctions corresponding to different eigenvalues are orthogonal** is a very general property, encountered in a much more general class of equations. These are called **Sturm-Liouville equations** and have the general form:

$$\frac{d}{dx}\left(p(x)\frac{du}{dx}\right) + q(x)u(x) + \lambda \rho(x) u(x) = 0 \tag{3}$$

where $x \in [a, b]$ (usually we chose $a = 0$, but it can have any value) and **homogeneous** boundary conditions:

$$\alpha_1 u(a) + \alpha_2 \frac{du}{dx}|_{x=a} = 0; \qquad \beta_1 u(b) + \beta_2 \frac{du}{dx}|_{x=b} = 0. \tag{4}$$

Of course, if $\alpha_2 = \beta_2$, the BC reduce to simple Dirichlet BC, while if $\alpha_1 = \beta_1 = 0$ they reduce to von Neumann BC. In other words, these are general enough to cover all possible homogeneous BC.

In Eq. (3), λ is the eigenvalue – it's a quantity whose allowed values are determined by the requirement that the BC conditions be satisfied. Note that our usual equation corresponds to the simplest possible choice $p(x) = \rho(x) = 1; q(x) = 0$ and we denoted $\lambda = k^2$ because of its units in this case. This reduces the general equation to our initial Eq. (1).

If $p(x), \rho(x)$ are positive, continuous functions on the $[a, b]$ interval, and moreover dp/dx is also continuous, this is called a *regular* Sturm-Liouville equation, and it has certain very useful properties. Before discussing them, let me make a few comments:

• First, you might wonder why should we bother with such a complicated equation, since we have never needed to solve anything like it. Well, in fact, if you look back at our derivation of the general form of the heat equation in 1D, we found:

$$\frac{\partial}{\partial x}\left(k(x)\frac{\partial u(x,t)}{\partial x}\right) + Q_{gen}(x,t) + \beta(x)\left[u(x,t) - T_0\right] = \rho(x)c_v(x)\frac{\partial u(x,t)}{\partial t}.$$

Here, the second term is related to the energy generated per unit time and volume inside the sample, while the 3rd was the heat that escapes through the lateral surface area, which we argues is generally proportional to the difference in temperature between the sample and the outside environment. Of course, if we put both these terms to zero, and assume that the heat conductivity k, the density ρ and the specific heat c_v are all constants (i.e., the material is homogeneous), then we recover our usual simplest equation $\frac{\partial^2 u}{\partial x^2} = \frac{1}{\kappa}\frac{\partial u}{\partial t}$.

However, it is also clear that if the material is not homogeneous and moreover, if it looses heat through its walls, than the homogeneous part of this equation is:

$$\frac{\partial}{\partial x}\left(k(x)\frac{\partial u(x,t)}{\partial x}\right) + \beta(x)u(x,t) = \rho(x)c_v(x)\frac{\partial u(x,t)}{\partial t}$$

Supposing we already dealt with the steady state solution, we would then need to solve for a transient solution $u_t(x,t) = X(x)T(t)$ which satisfies this general equation, plus homogeneous boundary conditions. This would lead to:

$$\frac{dT}{dt} = -\lambda T \to T(t) = e^{-\lambda t}$$

where we know that only values $\lambda > 0$ are of interest, since these solutions must go to zero as $t \to \infty$; and

$$\frac{d}{dx}\left(k(x)\frac{dX}{dx}\right) + \beta(x)X(x) = -\lambda\rho(x)c_v(x)X(x)$$

which has exactly the general form of the Sturm-Liouville equation, if we identify $k(x) \to p(x)$; $\beta(x) \to q(x)$; $\rho(x)c_v(x) \to \rho(x)$. Note, moreover, than in this case we are certain that $p(x), \rho(x)$ of the ST equation are continuous and positive functions, since they are related to material parameters which certainly have these properties. So if we want to solve the general heat equation, we do encounter precisely these kinds of equations, with precisely these kinds of boundary conditions.

• It can be shown that any second order ODE can be rewritten in the SL form of Eq. (3) (see textbook, section 17.4.2). However, the resulting $p(x), q(x)\rho(x)$ may not fulfil these conditions, so the SL equation is not necessarily regular. In that case, some of the properties we'll be discussing now may not hold!

A regular SL equation has the following properties:

1. All its eigenvalues are *real* numbers. I will not prove this, you will do it in your linear algebra course, where you will show that the operator acting on $X(x)$ is hermitian, and that any hermitian operator has real eigenvalues (see section 17.4.1. for a condensed proof).

2. There are an infinite number of eigenvalues, $\lambda_1 < \lambda_2 < ....$ Moreover, the eigenfunction $X_n(x)$ corresponding to the eigenvalue λ_n has precisely $n-1$ zeros inside the interval of interest $[a, b]$ (endpoints excluded).

I will not prove this either, but you can easily convince yourself that all cases we've studied had this property. This is most evident for the simplest case with Dirichlet BC, for $x \in [0, b]$, when we found $\lambda = k_n^2, k_n = \frac{n\pi}{b}, n = 1, 2, ...$ and $X_n(x) = \sin(k_n x)$.

3. Eigenfunctions corresponding to different eigenvalues are orthogonal, i.e.

$$\lambda_n \neq \lambda_m \rightarrow \int_a^b dx \rho(x) X_n(x) X_m(x) = 0$$

Note that we always integrate over the interval of interest; and that in general the function $\rho(x)$, which is called "the weight", enters in this condition. Of course, since for Eq. (1) $\rho(x) = 1$, then Eq. (2) is just a particular case of this general property.

Let's prove this. The equations satisfied by X_n and X_m are:

$$\frac{d}{dx}\left(p(x)\frac{dX_n}{dx}\right) + q(x)X_n(x) = -\lambda_n \rho(x) X_n(x) \tag{5}$$

$$\frac{d}{dx}\left(p(x)\frac{dX_m}{dx}\right) + q(x)X_m(x) = -\lambda_m \rho(x) X_m(x) \tag{6}$$

Of course, the eigenfunctions satisfy the BC as well, i.e.:

$$\alpha_1 X_n(a) + \alpha_2 \frac{dX_n}{dx}|_{x=a} = 0; \qquad \beta_1 X_n(b) + \beta_2 \frac{dX_n}{dx}|_{x=b} = 0$$

and

$$\alpha_1 X_m(a) + \alpha_2 \frac{dX_m}{dx}|_{x=a} = 0; \qquad \beta_1 X_m(b) + \beta_2 \frac{dX_m}{dx}|_{x=b} = 0$$

Note that we can combine the two left-end conditions into:

$$X_n(a)\frac{dX_m}{dx}|_{x=a} = X_m(a)\frac{dX_n}{dx}|_{x=a} \tag{7}$$

(just eliminate α_1, α_2 from the equations, knowing that the cannot possibly both be zero, since then we would have no BC). Similarly, on the other end, after getting rid of β's, we find:

$$X_n(b)\frac{dX_m}{dx}|_{x=b} = X_m(b)\frac{dX_n}{dx}|_{x=b} \tag{8}$$

We are now ready to proceed. We multiply Eq. (5) by $X_m(x)$, Eq. (6) by $X_n(x)$, subtract the two, and integrate the result from a to b (where both these equations hold). Note that the terms proportional to $q(x)$ cancel out. We are left with:

$$\int_a^b dx \left[X_m(x)\frac{d}{dx}\left(p(x)\frac{dX_n}{dx}\right) - X_n(x)\frac{d}{dx}\left(p(x)\frac{dX_m}{dx}\right)\right] = (\lambda_m - \lambda_n)\int_a^b \rho(x)X_n(x)X_m(x)$$

Here's the plan. If we can show that the LHS equals zero, then it follows immediately that for $\lambda_n \neq \lambda_m$, the integral on the RHS must be zero. In other words, the desired orthogonality condition. So let's show that the LHS vanishes. First, I will do an integration by parts:

$$X_m(x)\frac{d}{dx}\left(p(x)\frac{dX_n}{dx}\right) = \frac{d}{dx}\left(p(x)X_m(x)\frac{dX_n}{dx}\right) - p(x)\frac{dX_m}{dx}\frac{dX_n}{dx}$$

We do the same for the other term. When we subtract, we see that the latter terms cancel out, so we are left with:

$$\int_a^b dx \left[\frac{d}{dx}\left(p(x)X_m(x)\frac{dX_n}{dx}\right) - \frac{d}{dx}\left(p(x)X_n(x)\frac{dX_m}{dx}\right)\right] = p(x)\left[X_m(x)\frac{dX_n}{dx} - X_n(x)\frac{dX_m}{dx}\right]_a^b = 0$$

after using Eq. (7) and (8). So this orthogonality is always there. You can see that we can run into problems if $p(x)$ is singular either at $x = a$ or $x = b$, but this is certainly not the case for a regular SL problem.

4. Any "well-behaved" function $f(x)$ can be decomposed in a linear combination of these eigenfunctions over the $[a, b]$ interval, i.e. this set is *complete*:

$$f(x) = \sum_{n=1}^{\infty} a_n X_n(x)$$

The coefficients can be found from the orthogonality equation, by multiplying both sides by $\rho(x)X_m(x)$ and integrating, which leads to:

$$a_m = \frac{\int_a^b dx \rho(x) f(x) X_m(x)}{\int_0^a dx \rho(x) [X_m(x)]^2}, (\forall) m = 1, 2, ...$$

Note that we need to introduce the weight $\rho(x)$ into the integrals as well, otherwise the orthogonality does not hold.

Essentially, you can think of all these results as generalization of the Fourier series, except that the functions $X_m(x)$ can be a lot more complicated than simple sin/cosine functions that appear in Fourier series. Just like for Fourier series, one has to be a bit careful with $f(x)$ – it certainly shouldn't do anything too crazy, like infinite discontinuities etc. But since the functions we encounter in physics problems are usually well-enough behaved, we are generally safe.

One more comment: if you've learned quantum mechanics (or if not, when you will) these sort of discussions about orthogonal eigenfunctions and complete sets etc should be very familiar. There should be no surprise there, since we've seen that the heat equation and the Schrödinger equation have many similarities.