Sturm–Liouville Problems

More general eigenvalue problems

So far all of our example PDEs have led to separated equations of the form $X'' + \omega^2 X = 0$, with standard Dirichlet or Neumann boundary conditions. Not surprisingly, more complicated equations often come up in practical problems. For example, if the medium in a heat or wave problem is spatially inhomogeneous,* the relevant equation may look like

$$X'' - V(x)X = -\omega^2 X$$

for some function V, or even

$$a(x)X'' + b(x)X' + c(x)X = -\omega^2 X.$$

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* That is, the density, etc., vary from point to point. This is not the same as "nonhomogeneous" in the sense of the general theory of linear differential equations.

Also, if the boundary in a problem is a circle, cylinder, or sphere, the solution of the problem is simplified by converting to polar, cylindrical, or spherical coordinates, so that the boundary is a surface of constant radial coordinate. This simplification of the boundary conditions is bought at the cost of complicating the differential equation itself: we again have to deal with ODEs with nonconstant coefficients, such as

$$\frac{d^2R}{dr^2} + \frac{1}{r}\frac{dR}{dr} - \frac{n^2}{r^2}R = -\omega^2 R.$$

The good news is that many of the properties of Fourier series carry over to these more general situations. As before, we can consider the *eigenvalue problem* defined by such an equation together with appropriate boundary conditions: Find all functions that satisfy the ODE (for *any* value of ω) and also satisfy the boundary conditions. And it is still true (under certain conditions) that the set of all eigenfunctions is *complete*: *Any* reasonably well-behaved function can be expanded as an infinite series where each term is proportional to one of the

eigenfunctions. This is what allows arbitrary data functions in the original PDE to be matched to a sum of separated solutions! Also, the eigenfunctions are *orthogonal* to each other; this leads to a simple formula for the coefficients in the eigenfunction expansion, and also to a Parseval formula relating the norm of the function to the sum of the squares of the coefficients.

Orthonormal bases

Consider an interval $[a, b]$ and the real-valued (or complex-valued) functions defined on it. A sequence of functions $\{\phi_n(x)\}$ is called *orthogonal* if

$$\int_a^b \phi_n(x)^* \, \phi_m(x) \, dx = 0 \quad \text{whenever } m \neq n.$$

It is called *orthonormal* if, *in addition*, $\displaystyle\int_a^b |\phi_n(x)|^2 \, dx = 1.$

This normalization condition is merely a convenience; the important thing is the orthogonality. If we are lucky enough to have an orthogonal set, we can always convert it to an orthonormal set by dividing each function by the square root of its normalization integral:

$$\psi_n(x) \equiv \frac{\phi_n(x)}{\sqrt{\int_a^b |\phi_n(z)|^2\, dz}} \;\Rightarrow\; \int_a^b |\psi_n(x)|^2\, dx = 1.$$

However, in certain cases this may make the formula for ψ_n more complicated, so that the redefinition is hardly worth the effort. A prime example is the eigenfunctions in the Fourier sine series:

$$\phi_n(x) \equiv \sin nx \;\Rightarrow\; \int_0^\pi |\phi_n(x)|^2\, dx = \frac{\pi}{2}\,;$$

therefore,

$$\psi_n(x) \equiv \sqrt{\frac{2}{\pi}}\, \sin nx$$

are the elements of the orthonormal basis. (This is the kind of normalization often used for the Fourier sine *transform*, as we have seen.) A good case can be made, however, that normalizing the eigenfunctions is more of a nuisance than a help in this case; most people prefer to put the entire $2/\pi$ in one place rather than put half of it in the Fourier series and half in the cofficient formula.

Now let $f(x)$ be an arbitrary (nice) function on $[a, b]$. *If* f has an expansion as a linear combination of the ϕ's,

$$f(x) = \sum_{n=1}^{\infty} c_n \phi_n(x),$$

then

$$\int_a^b \phi_m(x)^* \, f(x) \, dx = \sum_{n=1}^{\infty} c_n \int_a^b \phi_m(x)^* \, \phi_n(x) \, dx = c_m \int_a^b |\phi_m(x)|^2 \, dx$$

by orthogonality. If the set is orthonormal, this just says

$$\boxed{c_m = \int_a^b \phi_m(x)^*\, f(x)\, dx.} \qquad (\P)$$

(In the rest of this discussion, I shall assume that the orthogonal set is orthonormal. This greatly simplifies the formulas of the general theory, even while possibly complicating the expressions for the eigenfunctions in any particular case.)

Remark: The integral on the right side of (¶) is called the *inner product* of ϕ_m and f and is often written as $\langle \phi_m, f \rangle$. It can be thought of as the generalization to an infinite-dimensional and complex vector space of the familiar dot product of vectors in $\mathbf{R}^3$. Then the normalization integral $\int |\phi_n|^2\, dx = \langle \phi_n, \phi_n \rangle \equiv \|\phi_n\|^2$ is the analog of the square of the *length* of a vector, and the *distance* between two vectors f and g is $\|f - g\|$, as applied in the next two paragraphs. For more on this linear-algebra analogy, see pp. 168–169 in Appendix B of the notes (pp.

26–27 of the `.pdf` file). The two previous pages of that Appendix give a simple example of a complete set of functions and a set that fails to be complete because some vectors have been left out.

It can easily be shown (just as for Fourier series) that

$$\boxed{\int_a^b |f(x)|^2\,dx = \sum_{n=1}^{\infty} |c_n|^2.}$$

This is the *Parseval equation* associated to this orthonormal set. Furthermore, if f is *not* of the form $\sum_{n=1}^{\infty} c_n\phi_n(x)$, then

$$\sum_{n=1}^{\infty} |c_n|^2 < \int_a^b |f(x)|^2\,dx \tag{1}$$

(called *Bessel's inequality*), and (2) the *best approximation* to $f(x)$ of the form $\sum c_n\phi_n(x)$ is the one where the coefficients are computed by formula (¶). These

last two statements remain true when $\{\phi_n\}$ is a *finite* set — in which case, obviously, the probability that a given f will not be exactly a linear combination of the ϕ's is greatly increased. The precise meaning of (2) is that the choice (¶) of the c_n minimizes the integral

$$\int_a^b \left| f(x) - \sum_{n=1}^{\infty} c_n \phi_n(x) \right|^2 dx.$$

That is, we are talking about *least squares approximation*. It is understood in this discussion that f itself is square-integrable on $[a, b]$. Recall that the space of such functions is called L^2 (or, more specifically, $L^2(a, b)$).

Now suppose that *every* square-integrable f is the limit of a series $\sum_{n=1}^{\infty} c_n \phi_n$. (This series is supposed to converge "in the mean" — that is, the least-squares integral

$$\int_a^b \left| f(x) - \sum_{n=1}^{M} c_n \phi_n(x) \right|^2 dx$$

for a partial sum approaches 0 as $M \to \infty$.) Then $\{\phi_n\}$ is called a *complete set* or an *orthonormal basis*. This is the analogue of the mean convergence theorem for Fourier series. Under certain conditions there may also be pointwise or uniform convergence theorems, but these depend more on the special properties of the particular functions ϕ being considered.

So far this is just a definition, not a theorem. To guarantee that our orthonormal functions form a basis, we have to know where they came from. The miracle of the subject is that the eigenfunctions that arise from variable-separation problems *do* form orthonormal bases:

Sturm–Liouville theory

Theorem: Suppose that the ODE that arises from some separation of vari-

ables is

$$\mathcal{L}[X] = -\lambda X \quad \text{on } (0, L), \tag{‡}$$

where $\mathcal{L}$ is an abbreviation for a second-order *linear differential operator*

$$\mathcal{L}[X] \equiv a(x)X'' + b(x)X' + c(x)X,$$

a, b, and c are continuous on $[0, L]$, and $a(x) > 0$ on $[0, L]$. Suppose further that

$$\int_0^L \big(\mathcal{L}[u](x)\big)^* \, v(x)\, dx = \int_0^L u(x)^* \, \big(\mathcal{L}[v](x)\big)\, dx \tag{†}$$

for all functions u and v satisfying the boundary conditions of the problem. (In terms of the inner product in L^2, this condition is just $\langle \mathcal{L}u, v\rangle = \langle u, \mathcal{L}v\rangle$. An operator satisfying this condition is called *self-adjoint* or *Hermitian*.[♯]) Then:

[♯] There is a technical distinction between these two terms, but it does not matter for regular Sturm–Liouville problems.

(1) All the eigenvalues λ are real (but possibly negative).

(2) The eigenfunctions corresponding to different λ's are orthogonal:

$$\int_0^L \phi_n(x)^* \, \phi_m(x) \, dx = 0 \quad \text{if } n \neq m.$$

(3) The eigenfunctions are complete. (This implies that the corresponding PDE can be solved for arbitrary boundary data, in precise analogy to Fourier series problems.)

The proof that a given $\mathcal{L}$ satisfies (†) (or doesn't satisfy it, as the case may be) involves integrating by parts twice. It turns out that (†) will be satisfied if $\mathcal{L}$ has the form

$$\frac{d}{dx} p(x) \frac{d}{dx} + q(x)$$

(with p and q real-valued and well-behaved, and $p(x) > 0$) and the boundary conditions are of the type

$$\alpha X'(0) - \beta X(0) = 0, \qquad \gamma X'(L) + \delta X(L) = 0$$

with α, etc., real.* Such an eigenvalue problem is called a *regular Sturm–Liouville problem*.

The proof of the conclusions (1) and (2) of the theorem is quite simple and is a generalization of the proof of the corresponding theorem for eigenvalues and eigenvectors of a *symmetric matrix* (which is proved in many physics courses and linear algebra courses). Part (3) is harder to prove, like the convergence theorems for Fourier series (which are a special case of it).

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* The reason for the minus sign in the first equation is to make true "property (7)" stated below.

Example: Convective boundary condition

The simplest nontrivial example of a Sturm–Liouville problem ("nontrivial" in the sense that it gives something other than a Fourier series) is the usual spatially homogeneous heat equation

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} \qquad (0 < x < L, \quad 0 < t < \infty),$$

with boundary conditions such as

$$u(0,t) = 0, \qquad \frac{\partial u}{\partial x}(L,t) + \beta u(L,t) = 0$$

and initial data

$$u(x,0) = f(x).$$

In a realistic problem, the zeros in the BC would be replaced by constants; as usual, we would take care of that complication by subtracting off a steady-state solution. Physically, the constant value of $\frac{\partial u}{\partial x}(L,t)+\beta u(L,t)$ is proportional to the temperature of the air (or other fluid medium) to which the right-hand endpoint of the bar is exposed; heat is lost through that end by convection, according to "Newton's law of cooling". Mathematically, such a BC is called a *Robin boundary condition*, as opposed to Dirichlet or Neumann.

The separation of variables proceeds just as in the more standard heat problems, up to the point

$$T(t) = e^{-\omega^2 t}, \qquad X(x) = \sin \omega x, \qquad \omega \equiv \sqrt{\lambda}.$$

To get the sine I used the boundary condition $X(0) = 0$. The other BC is

$$X'(L) + \beta X(L) = 0,$$

or

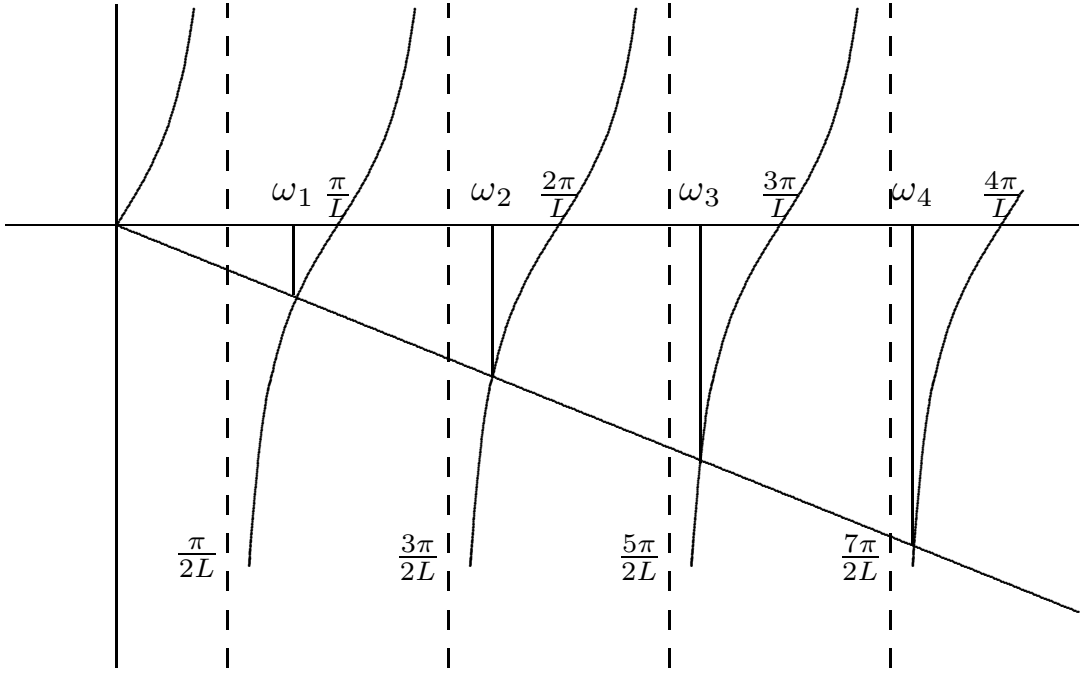
$$\frac{\omega}{\beta}\,\cos\omega L + \sin\omega L = 0, \qquad (*')$$

or

$$\tan\omega L = -\frac{1}{\beta}\,\omega. \qquad (*)$$

It is easy to find the *approximate* locations of the eigenvalues, $\lambda_n = {\omega_n}^2$, by graphing the two sides of $(*)$ (as functions of ω) and picking out the points of intersection. (In the drawing we assume $\beta > 0$.)

The nth root, ω_n, is somewhere between $\left(n - \frac{1}{2}\right)\frac{\pi}{L}$ and $\frac{n\pi}{L}$; as $n \to \infty$, ω_n becomes arbitrarily close to $\left(n - \frac{1}{2}\right)\frac{\pi}{L}$, the vertical asymptote of the tangent function. For smaller n one could guess ω_n by eye and then improve the guess by, for example, Newton's method. (Because of the violent behavior of tan near the asymptotes, Newton's method does not work well when applied to $(*)$; it is more fruitful to work with $(*')$ instead.)


ω_1 $\frac{\pi}{L}$
ω_2 $\frac{2\pi}{L}$
ω_3 $\frac{3\pi}{L}$
ω_4 $\frac{4\pi}{L}$
$\frac{\pi}{2L}$
$\frac{3\pi}{2L}$
$\frac{5\pi}{2L}$
$\frac{7\pi}{2L}$

To complete the solution, we write a linear combination of the separated solutions,

$$u(x,t) = \sum_{n=1}^{\infty} b_n \, \sin \omega_n x \, e^{-{\omega_n}^2 t},$$

and seek to determine the coefficients from the initial condition,

$$f(x) = u(x,0) = \sum_{n=1}^{\infty} b_n \, \sin \omega_n x.$$

This problem satisfies the conditions of the Sturm–Liouville theorem, so the eigenfunctions

$$\psi_n \equiv \sin \omega_n x$$

are guaranteed to be orthogonal. This can be verified by direct computation (making use of the fact that ω_n satisfies $(*)$). Thus

$$\int_0^L f(x) \, \sin \omega_m x \, dx = b_m \int_0^L \sin^2 \omega_m x \, dx.$$

However, the ψ_n have not been normalized, so we have to calculate

$$\int_0^L \sin^2 \omega_m x \, dx \equiv \|\psi_m\|^2$$

and divide by it. (This number is *not* just $\frac{1}{2}L$, as in the Fourier case.) Alternatively, we could construct *orthonormal* basis functions by dividing by the square root of this quantity:

$$\phi_n \equiv \frac{\psi_n}{\|\psi_n\|} \, .$$

Then the coefficient formula is simply

$$B_m = \int_0^L f(x) \, \phi_m(x) \, dx$$

(where $f(x) = \sum_m B_m \phi_m$, so $B_m = \|\psi_m\| b_m$).

The theorem also guarantees that the eigenfunctions are complete, so this solution is valid for any reasonable f. (Nevertheless, if $\beta < 0$ it is easy to overlook one of the normal modes and end up with an incomplete set by mistake. See Haberman, Figs. 5.8.2 and 5.8.3.)

More properties of Sturm–Liouville eigenvalues and eigenfunctions

Continuation of the theorem: For a *regular* Sturm–Liouville problem:

(4) For each eigenvalue λ there is at most one linearly independent eigenfunction. (*Note:* This is true only for the "regular" type of boundary conditions,

$$\alpha X'(0) - \beta X(0) = 0, \qquad \gamma X'(L) + \delta X(L) = 0.$$

For periodic boundary conditions there can be two independent eigenfunctions for the same λ, as we know from Fourier series.)

(5) λ_n approaches $+\infty$ as $n \to \infty$.

(6) $\phi_n(x)$ is real and has exactly $n-1$ zeros ("nodes") in the interval $(0, L)$ (endpoints not counted). The basic reason for this is that as λ increases, ϕ becomes increasingly concave and oscillatory. (This property, also, depends on regular boundary conditions. Clearly it is not true of the eigenfunctions e^{inx} in the full Fourier series.)

(7) If α, β, γ, δ, $p(x)$, and $-q(x)$ are all nonnegative, then the $\lambda_n \equiv {\omega_n}^2$ are all nonnegative. (*Corollary:* For the heat equation, the solution $u(x,t)$ approaches 0 as $t \to +\infty$ if all the eigenvalues are positive; it approaches a constant if $\omega = 0$ occurs.)

Note that parts (1) and (7) of the theorem make it possible to exclude the possibilities of complex and negative eigenvalues without a detailed study of the solutions of the ODE for those values of λ. In first learning about separation of

variables and Fourier series we did make such a detailed study, for the ODE $X'' = -\lambda X$, but I remarked that the conclusion could usually be taken for granted. (Indeed, Appendix A gives the proof of (1) and (7), specialized to $X'' = -\lambda X$.)

A good exercise: For a regular Sturm–Liouville problem with differential operator

$$\mathcal{L} = \frac{d}{dx} p(x) \frac{d}{dx} + q(x),$$

prove (†) and (7) along the lines previously indicated.

Nonstandard weight functions

Unfortunately, not all important problems fit exactly into this framework. Sometimes the ODE has the form (instead of (‡))

$$\mathcal{L}[X] = -\lambda r(x) X,$$

where $r(x) > 0$ on the interval and the operator is still of the form

$$\mathcal{L}[X] = \frac{d}{dx} p(x) \frac{d}{dx} + q(x).$$

(In particular, the radial operators that come from separating variables in polar and spherical coordinates are of this type.) From the point of view of general linear algebra it would make more sense to define a new operator

$$\mathcal{A}[X] \equiv \frac{\mathcal{L}[X]}{r(x)}, \qquad \mathcal{A}[X] = -\lambda X,$$

and to study its eigenvalues and eigenfunctions. However, it is $\mathcal{L}$, not $\mathcal{A}$, that satisfies the self-adjointness property (†) with respect to the standard inner product on functions in L^2. Instead, $\mathcal{A}$ is self-adjoint with respect to a *new* inner product,

$$\langle u, v \rangle_r \equiv \int_0^L u(x)^* v(x)\, r(x)\, dx\,;$$

$$\langle \mathcal{A}u, v\rangle_r = \langle u, \mathcal{A}v\rangle_r \,.$$

In this case, statement (2) of the theorem must be revised:

(2′) The eigenfunctions corresponding to different eigenvalues are orthogonal with respect to the *weight function* $r(x)$:

$$\langle \phi_n, \phi_m\rangle_r = \int_0^L \phi_n(x)^*\, \phi_m(x)\, r(x)\, dx = 0 \quad \text{if } n \neq m.$$

(Everything said previously about orthonormality can be generalized to the case of a nontrivial positive weight function. Thinking about the inner product abstractly, instead of as a certain integral, is very powerful here.)

In principle, a weight function can always be avoided by making a change of variable so that $dy = r(x)\, dx$. But in practice that may complicate the differential operator, making the cure at least as bad as the disease.

If one of the coefficient functions in the operator $\mathcal{L}$ violates a condition in the definition of a regular Sturm–Liouville problem at an endpoint (e.g., if $p(0) = 0$, or if $q(x) \to \infty$ as $x \to L$), or if the interval is infinite, then the problem is called *singular* (instead of regular). Many of the most important real-life cases *are* singular. Under these conditions the foregoing theory acquires complications, which I can discuss only very loosely here.

1. The set of eigenfunctions needed to expand an arbitrary function may depend on λ as a continuous variable, as in the case of the Fourier transform.

2. The boundary conditions needed to get an orthogonal and complete set of eigenfunctions may be of a different type. The critical condition that must be kept satisfied is (†). In particular, if one of the endpoints moves to infinity, then usually there is no boundary condition there of the type $\gamma X'(L) +$

$\delta X(L) = 0$; instead, one merely excludes solutions that grow exponentially fast at infinity. If all the remaining solutions go rapidly to zero at infinity, so that they are square-integrable, then the eigenfunction expansion will be a series, as in the regular problems. If the remaining solutions do not go to zero, then typically *all* of them are needed to form a complete set, and one has a situation like the Fourier transform.

Eigenfunctions, delta functions, and Green functions

Let's return to the regular case and assume that the eigenfunctions have been chosen orthonormal. (For simplicity I also assume that $r(x) = 1$; otherwise factors r and $1/r$ will show up in some of the formulas below.) We have an expansion formula

$$f(x) = \sum_{n=1}^{\infty} c_n \phi_n(x) \qquad (\sharp)$$

and a coefficient formula

$$c_m = \int_a^b \phi_m(z)^* \, f(z) \, dz. \qquad (\flat)$$

Substituting ($\flat$) into ($\sharp$) and interchanging the order of summation and integration yields

$$f(x) = \int_a^b dz \, f(z) \left[\sum_{n=1}^{\infty} \phi_n(x) \phi_n(z)^* \right].$$

In other words, when acting on functions with domain (a, b),

$$\boxed{\delta(x - z) = \sum_{n=1}^{\infty} \phi_n(x) \phi_n(z)^*.}$$

This is called the *completeness relation* for the eigenfunctions $\{\phi_n\}$, since it expresses the fact that the whole function f can be built up from the pieces $c_n \phi_n$. In the special case of the Fourier sine series, we looked at this formula earlier.

We can also substitute (♯) into (♭), getting

$$c_m = \sum_{n=1}^{\infty} c_n \left[\int_a^b \phi_m(x)^* \, \phi_n(x) \, dx \right].$$

This equation is equivalent to

$$\boxed{\int_a^b \phi_m(x)^* \, \phi_n(x) \, dx = \delta_{mn} \, ,}$$

where

$$\delta_{mn} \equiv \begin{cases} 1 & \text{if } m = n \\ 0 & \text{if } m \neq n. \end{cases}$$

(This is called the *Kronecker delta symbol*; it is the discrete analogue of the Dirac delta function — or, rather, Dirac's delta function is a continuum generalization

of it!) This *orthogonality relation* summarizes the fact that the ϕ's form an orthonormal basis.

Note that the completeness and orthogonality relations are very similar in structure. Basically, they differ only in that the variables x and n interchange roles (along with their alter egos, z and m). The different natures of these variables causes a sum to appear in one case, an integral in the other.

Finally, consider the result of substituting (♭) into the solution of an initial-value problem involving the functions ϕ_n. For example, for a certain heat-equation problem we would get

$$u(t,x) = \sum_{n=1}^{\infty} c_n \, \phi_n(x) \, e^{-{\omega_n}^2 t}.$$

This becomes

$$u(t,x) = \int_a^b dz\, f(z) \left[\sum_{n=1}^{\infty} \phi_n(x)\, \phi_n(z)^*\, e^{-{\omega_n}^2 t} \right].$$

Therefore, the Green function for that problem is

$$\boxed{G(x,z;t) = \sum_{n=1}^{\infty} \phi_n(x)\, \phi_n(z)^*\, e^{-{\omega_n}^2 t}.}$$

When $t = 0$ this reduces to the completeness relation, since

$$\lim_{t \downarrow 0} G(x,z;t) = \delta(x-z).$$

Similarly,

$$G(x,z;\lambda) = \sum_{n=1}^{\infty} \frac{\phi_n(x)\, \phi_n(z)^*}{{\omega_n}^2 - \lambda^2}$$

is the *resolvent kernel*, the Green function such that

$$u(x) = \int_0^L G(x, z; \lambda) g(z)\, dz$$

solves the nonhomogeneous ODE $\mathcal{L}[u] + \lambda^2 u = -g$ (if $r = 1$) with the given boundary conditions. (Our first Green function example constructed with the aid of the delta function, several sections back, was a resolvent kernel.)

It may be easier to solve for the Green functions directly than to sum the series in these formulas. In fact, such formulas are often used in the reverse direction, to obtain information about the eigenfunctions and eigenvalues from independently obtained information about the Green function.