Linear Differential Equations
Physics 129a
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1 Introduction

A common problem we are faced with is that of solving for u in

$$Lu = g, \tag{1}$$

where L is a linear differential operator. We address this problem in this note, including both some theoretical remarks and practical approaches. Some foundational background may be found in the notes on Hilbert Spaces and on Distributions.

We will denote here whatever Hilbert space we are working in by the symbol $\mathcal{H}$.

2 Self-adjoint Operators

In physics, we typically encounter problems involving Hermitian operators:

Definition: If L is an operator with domain D_L, and

$$\langle Lu|v\rangle = \langle u|Lv\rangle \tag{2}$$

for all $u, v \in D_L$, then L is called a **Hermitian operator**.

The common appearance of Hermitian operators in physics has to do with the reality of their eigenvalues, e.g., the eigenvalues of a Hermitian matrix are real.

However, in general the specification that an operator be Hermitian may not be restrictive enough, once we consider differential operators on function spaces. We define the notion of the adjoint of an operator:

Definition: Given an operator L, with domain D_L such that D_L is dense in $\mathcal{H}$ (i.e., $\bar{D}_L = \mathcal{H}$), the **adjoint** $L^\dagger$ of L is defined according to:

$$\langle L^\dagger u|v\rangle = \langle u|Lv\rangle, \quad \forall v \in D_L. \tag{3}$$

It may be remarked that the domain, $D_{L^\dagger}$, of $L^\dagger$ is not necessarily identical with D_L.

Definition: If $L^\dagger = L$, which means:

$$\begin{aligned} D_{L^\dagger} &= D_L, \quad \text{and} && (4)\\ L^\dagger u &= Lu, \quad \forall u \in D_L, && (5) \end{aligned}$$

then L is said to be **self-adjoint**.

Note that a self-adjoint operator is Hermitian, but the converse may not hold, due to the added condition on domain.

Let us remark further on the issue of domain. A differential equation is not completely specified until we give certain boudary conditions which the solutions must satisfy. Thus, for a function to belong to D_L, not only must the expression Lu be defined, but u must also satisfy the boundary conditions. If the boundary conditions are too restrictive, then we might have $D_L \subset D_L^\dagger$, but $D_L^\dagger \neq D_L$, so that a Hermitian operator may not be self-adjoint.

For example, consider the "momentum operator", $p = -id/dx$, in quantum mechanics. Suppose x is confined to the region $[a, b]$, and we'll leave the boundary conditions to be specified. Supposing u and v to be continuous functions, we may evaluate, using integration by parts:

$$\begin{aligned} \langle u|pv\rangle &= \int_a^b u^*(x)\frac{1}{i}\frac{dv}{dx}(x)dx && (6)\\ &= \frac{1}{i}u^*(x)v(x)\Big|_a^b - \int_a^b \frac{1}{i}\frac{du^*}{dx}(x)v(x)dx && (7)\\ &= \frac{1}{i}\left[u^*(b)v(b) - u^*(a)v(a)\right] + \langle qu|v\rangle && (8)\\ &= \langle p^\dagger u|v\rangle, && (9) \end{aligned}$$

where we define the adjoint operator in the last line. Thus,

$$\langle p^\dagger u|v\rangle - \langle qu|v\rangle = \langle (p^\dagger - q)u|v\rangle = \frac{1}{i}\left[u^*(b)v(b) - u^*(a)v(a)\right]. \qquad (10)$$

We have used the symbol q instead of p here to indicate the operator $-id/dx$, but without implication that the domain of q has the same boundary conditions as p. That is, it may be that D_p is a proper subset of D_q. If p is to be Hermitian, we must have that the integrated part vanishes:

$$u^*(b)v(b) - u^*(a)v(a) = 0 \quad \forall u, v \in D_p. \qquad (11)$$

Also, equation 10 holds for all $v \in D_p$. If D_p is dense in $\mathcal{H}$, then the only vector orthogonal to all v is the null vector. Hence, $p^\dagger u = qu$ for all $u \in D_q \cap D_{p^\dagger}$.

Let's try a couple of explicit boundary conditions:

1. Suppose $D_p = \{v|v$ is continuous, and $v(a) = v(b)\}$, that is, a periodic boundary condition. Then we can have

$$\langle p^\dagger u|v\rangle = \langle qu|v\rangle, \quad \forall v \in D_p, \tag{12}$$

if and only if $u(a) = u(b)$ in order that the integrated part vanishes. Hence $D_{p^\dagger} = D_p$ and we have a self-adjoint operator.

2. Now suppose the boundary condition on v is $v(a) = v(b) = 0$. In this case, u can be any differentiable function and p will still be a Hermitian operator. We have that $D_{p^\dagger} \neq D_p$, hence p is not self-adjoint.

Why are we worrying about this distinction between Hermiticity and self-adjointness? Stay tuned.

Recall that we are interested in solving the equation $Lu(x) = g(x)$ where L is a differential operator, and $a \leq x \leq b$. One approach to this is to find the "inverse" of L, called the Green's function:

$$L_x G(x,y) = \delta(x-y), \qquad a \leq x, y \leq b. \tag{13}$$

Note that we put an "x" subscript on L when we need to be clear about the variable involved.

We may show how u is obtained with the above $G(x,y)$:

$$\begin{aligned} g(x) &= \int_a^b \delta(x-y)g(y)dy \\ &= \int_a^b L_x G(x,y)g(y)dy \\ &= L_x\left[\int_a^b G(x,y)g(y)dy\right] \\ &= L_x u(x), \end{aligned} \tag{14}$$

where

$$u(x) = \int_a^b G(x,y)g(y)dy, \tag{15}$$

is the desired solution.

Now also consider the eigenvalue problem:

$$L_x u(x) = \lambda u(x). \tag{16}$$

If we know $G(x,y)$ then we may write:

$$u(x) = \int_a^b G(x,y)\lambda u(y)dy, \tag{17}$$

or,

$$\int_a^b G(x,y)u(y)dy = \frac{u(x)}{\lambda}, \tag{18}$$

as long as $\lambda \neq 0$. Thus, the eigenvectors of the (nice) integral operator are the same as those of the (unnice) differential operator and the corresponding eigenvalues (with redefinition of the integral operator eigenvalues from that in the Integral Note) are the inverses of each other.

We have the theorem:

Theorem: The eigenvectors of a compact, self-adjoint operator form a complete set (when we include eigenvectors corresponding to zero eigenvalues).

Our integral operator is self-adjoint if $G(x,y) = G^*(y,x)$, since then

$$\int_a^b \int_a^b \phi^*(x)G(x,y)\psi(y)dxdy = \int_a^b \int_a^b \left[G(y,x)\phi(x)\right]^* \psi(y)dxdy, \tag{19}$$

for any vectors $\phi, \psi \in \mathcal{H}$. That is, $\langle\phi|G\psi\rangle = \langle G\phi|\psi\rangle$, in accordance with the definition of self-adjointness. Note that there are no sticky domain questions here, if we take our Hilbert space to be the space of square-integrable functions on (a,b), denoted $L^2(a,b)$. Our integral operator is also compact, if

$$\int_a^b \int_a^b |G(x,y)|^2 \, dxdy < \infty. \tag{20}$$

Thus, if a Green's function $G(x,y)$ associated with a given differential operator L is compact and self-adjoint, then by appending to the set of eigenvectors of the integral operator the linearly independent solutions of the homogeneous differential equation

$$L\beta_0(x) = 0, \tag{21}$$

we have a complete set of eigenvectors. That is, the eigenfunctions of L span $L^2(a,b)$. In practice, we have that one means of obtaining the eigenfunctions of L is to find G and then find the eigenfunctions of the integral equation.

Our problem reduces in some sense to one of finding the conditions on L so that G is self-adjoint and compact. If L is self-adjoint, then so is G, but remember the added considerations we had to deal with for the self-adjointness of L. If $[a,b]$ is a finite range, then the theory of ordinary differential equations guarantees that G is compact. If $[a,b]$ is infinite, then we must examine the particular case. However, for many important cases in physics, G is compact here as well.

Suppose that L is a Hermitian operator. We may demonstrate that its eigenvalues are real, and that eigenvectors corresponding to distinct eigenvalues are orthogonal: With eigenvectors:

$$L|\beta_i\rangle = \lambda_i|\beta_i\rangle, \tag{22}$$

we have

$$\langle\beta_j|L\beta_i\rangle = \lambda_i\langle\beta_j|\beta_i\rangle. \tag{23}$$

We also have:

$$\langle L\beta_j|\beta_i\rangle = \lambda_j^*\langle\beta_j|\beta_i\rangle. \tag{24}$$

But $\langle\beta_j|L\beta_i\rangle = \langle L\beta_j|\beta_i\rangle$ by Hermiticity. Hence,

$$(\lambda_i - \lambda_j^*)\langle\beta_j|\beta_i\rangle = 0. \tag{25}$$

If $i = j$, then $\lambda_i = \lambda_i^*$, that is, the eigenvalues of a Hermitian operator are real. If $i \neq j$ and $\lambda_i \neq \lambda_j$ then $\langle\beta_j|\beta_i\rangle = 0$, that is, the eigenvectors corresponding to distinct eigenvalues are orthogonal. If $i \neq j$ but $\lambda_i = \lambda_j$ then we may still construct an orthonormal basis of eigenfunctions by using the Gram-Schmidt algorithm. Thus, we may always pick our eigenfunctions of a Hermitian operator to be orthonormal:

$$\langle\beta_i|\beta_j\rangle = \delta_{ij}. \tag{26}$$

Further, this set is complete, at least if $[a, b]$ is finite and L is self-adjoint (other cases require further examination). We'll usually assume completeness of the set of eigenfunctions.

Now let us write our inhomogeneous differential equation in a form suggestive of our study of integral equations:

$$Lu(x) - \lambda u(x) = g(x). \tag{27}$$

Expand in eigenfunctions:

$$|u\rangle = \sum_i |\beta_i\rangle\langle\beta_i|u\rangle \tag{28}$$

$$|g\rangle = \sum_i |\beta_i\rangle\langle\beta_i|g\rangle. \tag{29}$$

Substituting into the differential equation:

$$\sum_i (L - \lambda)|\beta_i\rangle\langle\beta_i|u\rangle = \sum_i |\beta_i\rangle\langle\beta_i|g\rangle. \tag{30}$$

Since $L|\beta_i\rangle = \lambda_i|\beta_i\rangle$, we obtain

$$\langle\beta_i|u\rangle = \frac{\langle\beta_i|g\rangle}{\lambda_i - \lambda}, \tag{31}$$

if $\lambda \neq \lambda_i$. Thus,

$$|u\rangle = \sum_i |\beta_i\rangle \frac{\langle\beta_i|g\rangle}{\lambda_i - \lambda} = \sum_i \frac{\beta_i(x)}{\lambda_i - \lambda} \int \beta_i^*(y) g(y) dy. \tag{32}$$

This is a familiar-looking result considering our study of integral equations. If $\lambda = \lambda_i$, we will have a solution only if $\langle\beta_i|g\rangle = 0$.

As in the study of integral equations, we are led to the "alternative theorem":

Theorem: Either $(L - \lambda)u = g$, where L is a compact linear operator, has a unique solution:

$$|u\rangle = \sum_i |\beta_i\rangle \frac{\langle\beta_i|g\rangle}{\lambda_i - \lambda}, \tag{33}$$

or the homogeneous equation $(L - \lambda)u = 0$ has a solution (i.e., λ is an eigenvalue of L). In this latter case, the original inhomogeneous equation has a solution if and only if $\langle\beta_i|g\rangle = 0$ for all eigenvectors β_i belonging to eigenvalue λ. If so, the solution is not unique:

$$|u\rangle = \sum_{i,\lambda_i \neq \lambda} |\beta_i\rangle \frac{\langle\beta_i|g\rangle}{\lambda_i - \lambda} + \sum_{i,\lambda_i = \lambda} c_i|\beta_i\rangle, \tag{34}$$

where the c_i are arbitrary constants.

The Green's function for the operator $L - \lambda$,

$$u(x) = \int_a^b G(x, y) g(y) dy, \tag{35}$$

is given by:

$$G(x, y) = \sum_i \frac{|\beta_i\rangle\langle\beta_i|}{\lambda_i - \lambda} = \sum_i \frac{\beta_i(x)\beta_i^*(y)}{\lambda_i - \lambda}. \tag{36}$$

We may make the following remarks about Green's functions:

1. If λ is real, then $G(x, y) = G^*(y, x)$, since λ_i is real. If the eigenfunctions are real, then G is real symmetric.

2. $G(x, y)$ satisfies the boundary conditions of the differential equation, since the eigenfunctions do.

3. Since
$$g(x) = (L - \lambda)u(x) = (L_x - \lambda)\int G(x,y)g(y)dy, \tag{37}$$
and $g(x) = \int \delta(x-y)g(y)dy$, we have that the Green's function satisfies the "differential equation" (an operator equation):
$$L_x G(x,y) - \lambda G(x,y) = \delta(x-y). \tag{38}$$
Thus, G may be regarded as the solution (including boundary conditions) to the original problem, but for a "point source" (rather than the "extended source" described by $g(x)$).

Thus, in addition to the method of finding the eigenfunctions, we have a second promising practical approach to finding the Green's function, that of solving the differential equation
$$(L_x - \lambda)G(x,y) = \delta(x-y). \tag{39}$$
We will return to this idea shortly.

3 The Sturm-Liouville Problem

Consider the general linear second order homogeneous differential equation in one dimension:
$$a(x)\frac{d^2}{dx^2}u(x) + b(x)\frac{d}{dx}u(x) + c(x)u(x) = 0. \tag{40}$$
Under quite general conditions, as the reader may discover, this may be written in the form of a differential equation involving a self-adjoint (with appropriate boundary conditions) **Sturm-Liouville operator**:
$$Lu = 0, \tag{41}$$
where
$$L = \frac{d}{dx}p(x)\frac{d}{dx} - q(x). \tag{42}$$

We are especially interested in the "eigenvalue equation" corresponding to L, in the form:
$$Lu + \lambda wu = 0, \tag{43}$$
or
$$\frac{d}{dx}\left[p(x)\frac{du}{dx}(x)\right] - q(x)u(x) + \lambda w(x)u(x) = 0. \tag{44}$$
Here, λ is an "eigenvalue" for "eigenfunction" $u(x)$, satisfying the boundary conditions. Note the sign change from the eigenvalue equation we often write, this is just a convention. The function $w(x)$ is a real, non-negative "weight function".

3.1 An Example

Let's consider a simple example:

$$L = \frac{d^2}{dx^2} + 1, \quad x \in [0, \pi], \tag{45}$$

with homogeneous boundary conditions $u(0) = u(\pi) = 0$. This is of Sturm-Liouville form with $p(x) = 1$ and $q(x) = -1$. Suppose we wish to solve the inhomogeneous equation:

$$Lu = \cos x. \tag{46}$$

A solution to this problem is $u(x) = \frac{x}{2} \sin x$, as may be readily verified, including the boundary conditions. But we notice also that

$$\frac{d^2}{dx^2} \sin x + \sin x = 0. \tag{47}$$

Our solution is not unique. The most general solution is

$$u(x) = \frac{x}{2} \sin x + A \sin x, \tag{48}$$

where A is an arbitrary constant.

Let's examine how this fits in with our theorems about expansions in terms of eigenfunctions, and perhaps imagine that the $\frac{x}{2} \sin x$ solution did not occur to us. We'll assert (and leave it to the reader to demonstrate) that our operator with these boundary conditions is self-adjoint. Thus, the eigenfunctions must form a complete set.

Consider $Lu_n = \lambda_n u_n$ and $Lu = f$. We expand:

$$u = \sum_n |u_n\rangle\langle u_n|u\rangle \tag{49}$$

$$f = \sum_n |u_n\rangle\langle u_n|f\rangle. \tag{50}$$

Thus, $Lu = f$ implies

$$u = \sum_n |u_n\rangle \frac{\langle u_n|f\rangle}{\lambda_n} \tag{51}$$

If $\lambda_n = 0$, then there is no solution unless $\langle u_n|f\rangle = 0$, in which case the solution is not unique.

Let us proceed to find the eigenfunctions. We may write $Lu_n = \lambda_n u_n$ in the form

$$u_n'' + (1 - \lambda_n)u_n = 0. \tag{52}$$

Solutions to this equation, satisfying the boundary conditions are

$$u_n(x) = A_n \sin nx, \quad n = 1, 2, 3, \ldots, \tag{53}$$

with $\lambda_n = 1 - n^2 = 0, -3, -8, -15, \ldots$. With $A_n = \sqrt{2/\pi}$, we have an orthonormal set.

The zero eigenvalue looks like trouble for equation 51. Either the solution to the problem $Lu = \cos x$ doesn't exist, or it is of the form:

$$u(x) = \sum_{n=2}^{\infty} \sqrt{\frac{2}{\pi}} \sin nx \frac{\int_0^\pi \sqrt{\frac{2}{\pi}} \sin ny \cos y dy}{1 - n^2} + C \sin x. \tag{54}$$

We add the last term, with C arbitrary, because "λ" $= \lambda_1 = 0$. We started the sum at $n = 2$ because of the difficulty with $\lambda_1 = 0$. However, we must check that this is permissible:

$$\int_0^\pi \sin x \cos x dx = 0, \tag{55}$$

so far so good.

In general, we need, for $n = 2, 3, \ldots$:

$$\begin{aligned} I_n &\equiv \int_0^\pi \sin nx \cos x dx \\ &= \frac{1}{2} \int_0^\pi \left[\sin(n+1)x + \sin(n-1)x\right] dx \\ &= \begin{cases} 0 & n \text{ odd,} \\ \frac{2n}{n^2-1} & n \text{ even.} \end{cases} \end{aligned} \tag{56}$$

Then the solution is

$$\begin{aligned} u(x) &= \sum_{n=2,\text{even}}^{\infty} \frac{2}{\pi} \frac{1}{1-n^2} \frac{2n}{n^2-1} \sin nx + C \sin x \\ &= C \sin x - \frac{4}{\pi} \sum_{n=2,\text{even}}^{\infty} \frac{n}{(n^2-1)^2} \sin nx. \end{aligned} \tag{57}$$

But does the summation above give $\frac{x}{2} \sin x$? We should check that our two solutions agree. In fact, we'll find that

$$\frac{x}{2} \sin x \neq -\frac{4}{\pi} \sum_{n=2,\text{even}}^{\infty} \frac{n}{(n^2-1)^2} \sin nx. \tag{58}$$

But we'll also find that this is all right, because the difference is just something proportional to $\sin x$, the solution to the homogeneous equation. To answer this question, we evidently wish to find the sine series expansion of $\frac{x}{2}\sin x$:

$$f(x)=\sum_{n=1}^{\infty} a_n\sqrt{\frac{2}{\pi}}\sin nx, \tag{59}$$

where $f(x)=\frac{x}{2}\sin x$, and the interval of interest is $(0,\pi)$.

We need to determine the expansion coefficients a_n:

$$\begin{aligned}
a_n &= \sqrt{\frac{2}{\pi}}\int_0^\pi f(x)\sin nx dx\\
&= \frac{1}{\sqrt{2\pi}}\int_0^\pi x\sin x\sin nx dx\\
&= \frac{1}{\sqrt{8\pi}}\int_0^\pi x\left[\cos(n-1)x-\cos(n+1)x\right]dx\\
&= \frac{1}{\sqrt{8\pi}}\left\{x\left[\frac{\sin(n-1)x}{n-1}-\frac{\sin(n+1)x}{n+1}\right]_0^\pi-\int_0^\pi\left[\frac{\sin(n-1)x}{n-1}-\frac{\sin(n+1)x}{n+1}\right]dx\right\}\\
&= \begin{cases} 0 & n \text{ odd}, n\neq 1,\\ \frac{1}{\sqrt{2\pi}}\left[\frac{-4n}{(n^2-1)^2}\right] & n\geq 2, \text{ even.}\end{cases}
\end{aligned} \tag{60}$$

The a_1 coefficient we evaluate separately, finding

$$a_1=\frac{1}{\sqrt{2\pi}}\frac{\pi^2}{4}. \tag{61}$$

Thus, our expansion is

$$\frac{x}{2}\sin x=\frac{\pi}{4}\sin x-\frac{4}{\pi}\sum_{n=2,\text{even}}^{\infty}\frac{n}{(n^2-1)^2}\sin nx. \tag{62}$$

Our solution in terms of an expansion in eigenfunctions is correct.

Suppose, instead that we wished to solve

$$Lu=\cos x, \tag{63}$$

again with $L=\frac{d^2}{dx^2}+1$, and $x\in[0,\pi]$, but now with boundary conditions $u(0)=u'(0)=0$. Certainly the solution $u(x)=\frac{x}{2}\sin x$ still works, and satisfies the boundary conditions.

Let us try the eigenfunction expansion approach once more. Start with the eigenvalue equation:

$$u''+(1-\lambda)u=0. \tag{64}$$

If $\lambda=1$ then $u(x)=ax+b$. If $\lambda\neq 1$ then

$$u(x)=A\sin\sqrt{1-\lambda}x+B\cos\sqrt{1-\lambda}x. \tag{65}$$

The boundary condition $u(0) = 0$ implies $b = 0$ or $B = 0$, depending on λ. The boundary condition $u'(0) = 0$ implies $a = 0$ or $A = 0$, again depending on λ. There is no non-trivial solution to the eigenvalue equation with these boundary conditions! In particular, there is no non-trivial solution to the homogeneous equation $Lu = 0$, so the above solution must be unique.

We see that our attempt to solve this problem by expanding in eigenfunctions failed. What went wrong? The problem is that L is not self-adjoint, or even Hermitian, so our nice theorem does not apply. For L to be Hermitian, we must have

$$\langle Lu|v\rangle = \langle u|Lv\rangle \tag{66}$$

for all $u, v \in D_L$, that is, for all u, v satisfying the boundary conditions. Let's evaluate:

$$\begin{aligned}\langle Lu|v\rangle - \langle u|Lv\rangle &= \int_0^\pi \frac{d^2u^*}{dx^2}(x)v(x)dx - \int_0^\pi u^*(x)\frac{d^2v}{dx^2}(x)dx \\ &= \frac{du^*}{dx}(x)v(x)\Big|_0^\pi - u^*(x)\frac{dv}{dx}(x)\Big|_0^\pi \\ &= \frac{du^*}{dx}(\pi)v(\pi) - u^*(\pi)\frac{dv}{dx}(\pi). \end{aligned} \tag{67}$$

This is non-zero in general.

Can we still find a Green's function for this operator? We wish to find $G(x, y)$ such that:

$$\frac{\partial^2 G}{\partial x^2}(x, y) + G(x, y) = \delta(x - y). \tag{68}$$

For $x \neq y$, we have solution:

$$G(x, y) = \begin{cases} A(y)\sin x + B(y)\cos x, & x < y \\ C(y)\sin x + D(y)\cos x, & x > y. \end{cases} \tag{69}$$

The boundary conditions at $x = 0$ give us:

$$G(0, y) = 0 = B(y) \tag{70}$$

$$\frac{dG}{dx}(0, y) = 0 = A(y). \tag{71}$$

That is, $G(x, y) = 0$ for $x < y$. Notice that we have made no requirement on boundary conditions for y. Since L is not self-adjoint, there is no such constraint!

At $x = y$, G must be continuous, and its first derivative must have a discontinuity of one unit, so that we get $\delta(x-y)$ when we take the second derivative:

$$
\begin{aligned}
0 &= C(y)\sin y + D(y)\cos y && (72)\\
1 &= C(y)\cos y - D(y)\sin y. && (73)
\end{aligned}
$$

Thus, $C(y) = \cos y$ and $D(y) = -\sin y$, and the Green's function is:

$$
G(x,y) = \begin{cases} 0, & x < y \\ \sin x \cos y - \cos x \sin y, & x > y. \end{cases} \tag{74}
$$

Let's check that we can find the solution to the original equation $Lu(x) = \cos x$. It should be given by

$$
\begin{aligned}
u(x) &= \int_0^\pi G(x,y)\cos y dy \\
&= \int_0^x (\sin x \cos y - \cos x \sin y)\cos y dy \\
&= \frac{x}{2}\sin x. && (75)
\end{aligned}
$$

The lesson is that, even when the eigenvector approach fails, the method of Green's functions may remain fruitful.

3.2 Weights

We briefly discuss the "weight function" (or "density function") appearing in the Sturm-Liouville eigenvalue equation. Suppose u_i and u_j are solutions, corresponding to eigenvalues λ_i and λ_j:

$$
\begin{aligned}
Lu_i &= -\lambda_i w u_i, && (76)\\
Lu_j &= -\lambda_j w u_j && (77)
\end{aligned}
$$

Then,

$$
\begin{aligned}
\int u_j^* L u_i dx &= -\lambda_i \int u_j^* w u_i dx, && (78)\\
\int u_i (Lu_j)^* dx &= -\lambda_j^* \int u_j^* w u_i dx. && (79)
\end{aligned}
$$

where we have used the fact that $w(x)$ is real. By Hermiticity, the two lines above are equal, and we have:

$$
(\lambda_i - \lambda_j^*) \int u_j^* w u_i dx = 0. \tag{80}
$$

Considering $i = j$, the integral is positive (non-zero), hence the eigenvalues are real. With $i \neq j$, u_i and u_j are orthogonal when the weight function w is included, at least for $\lambda_i \neq \lambda_j$. When $\lambda_i = \lambda_j$ we may again use the Gram-Schmidt procedure, now including the wieght function, to obtain an orthogonal set.

Normalizing, we may express our orthonormality of eigenfunctions as:

$$\int u_j(x)u_i(x)w(x)dx = \delta_{ij}. \tag{81}$$

Note that, since $w(x) \geq 0$ (actually, we permit it to be zero only on a set of measure zero), this weighted integral defines a scalar product. We'll see several examples in the following section.

4 Some Important Sturm-Liouville Operators

Many problems in physics involve second order linear differential equations and can be put into Sturm-Liouville form. We give several important examples in this section.

4.1 Legendre Equation

When dealing with angular momentum in quantum mechanics, we encounter Legendre's equation:

$$(1 - x^2)\frac{d^2u}{dx^2} - 2x\frac{du}{dx} + \ell(\ell + 1)u = 0. \tag{82}$$

The typical situation is for x to be the cosine of a polar angle, and hence $|x| \leq 1$. When ℓ is an integer, the solutions are the Legendre polynomials $P_\ell(x)$ and the Legendre functions of the second kind $Q_\ell(x)$. These solutions may be obtained by assuming a series solution and substituting into the differential equation to discover the recurrence relation.

We may put the Legendre Equation in the Sturm-Liouville form by letting

$$\begin{aligned} p(x) &= 1 - x^2 & (83)\\ q(x) &= 0 & (84)\\ w(x) &= 1 & (85)\\ \lambda &= \ell(\ell + 1). & (86) \end{aligned}$$

4.2 Associated Legendre Equation

The Legendre equation above is a special case of the associated Legendre equation:

$$(1-x^2)\frac{d^2u}{dx^2} - 2x\frac{du}{dx} + \ell(\ell+1)u - \frac{m^2}{1-x^2}u = 0. \tag{87}$$

This may be put in Sturm-Liouville form the same as the Legendre equation, except now with

$$q(x) = \frac{m^2}{1-x^2}. \tag{88}$$

Again, this equation typically arises for $x = \cos\theta$. The additional term arises when the azimuthal symmetry is broken. That is, when dealing with the Laplacian in spherical coordinates, the term:

$$\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2} \to \frac{m^2}{1-\cos^2\theta} \tag{89}$$

when solving the partial differential equation by separation of variables. In this case ℓ is an non-negative integer, and m takes on values $-\ell, -\ell+1, \ldots, \ell$

The solutions are the associated Legendre polynomials $P_\ell^m(x)$, and series (singular at $|x| = 1$) $Q_\ell^m(x)$. The associated Legendre polynomials may be obtained from the Legendre polynomials according to:

$$P_\ell^m(x) = (-)^m(1-x^2)^{m/2}\frac{d^m}{dx^m}P_\ell(x). \tag{90}$$

4.3 Bessel Equation

While the Legendre equation appears when one applies separation of variables to the Laplacian in spherical coordinates, the Bessel equation shows up similarly when cylindrical coordinates are used. In this case, the interpretation of x is as a cylindrical radius, so typically the region of interest is $x \geq 0$. But the Bessel equation shows up in many places where it might not be so expected. The equation is:

$$x^2\frac{d^2u}{dx^2} + x\frac{du}{dx} + (x^2 - n^2)u = 0. \tag{91}$$

We could put this in Sturm-Liouville form by letting (noting that simply letting $p(x) = x^2$ doesn't work, we divide the equation by x):

$$\begin{aligned} p(x) &= x & (92)\\ q(x) &= -x & (93)\\ w(x) &= 1/x & (94)\\ \lambda &= -n^2. & (95) \end{aligned}$$

However, let's try another approach, motivated by an actual situation where the equation arises. Thus, suppose we are interested in solving the Helmholtz equation (or wave equation) in cylindrical coordinates:

$$\nabla^2\psi + k^2\psi = 0, \tag{96}$$

or

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial\psi}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2\psi}{\partial\theta^2} + \frac{\partial^2\psi}{\partial z^2} + k^2\psi = 0. \tag{97}$$

According to the method of separation of variables, we look for solutions of the form:

$$\psi(r,\theta,z) = R(r)\Theta(\theta)Z(z). \tag{98}$$

The general solution is constructed by linear combinations of such "separated" solutions.

Substituting the proposed solution back into the differential equation, and dividing through by ψ, we obtain:

$$\frac{1}{rR}\frac{d}{dr}\left(r\frac{dR}{dr}\right) + \frac{1}{r^2\Theta}\frac{d^2\Theta}{d\theta^2} + \frac{1}{Z}\frac{d^2Z}{dz^2} + k^2 = 0. \tag{99}$$

The third term does not depend on r or θ. It also cannot depend on z, since the other terms do not depend on z. Thus, the third term must be a constant, call it $\nu^2 - k^2$.

If we multiply the equation through by r^2, we now have an equation in two variables:

$$\frac{r}{R}\frac{d}{dr}\left(r\frac{dR}{dr}\right) + r^2\nu^2 + \frac{1}{\Theta}\frac{d^2\Theta}{d\theta^2} = 0. \tag{100}$$

The third term does not depend on r. It also cannot depend on θ, since the first two terms have no θ dependence. It must therefore be a constant, call it c^2. Then

$$\frac{d^2\Theta}{d\theta^2} = -c^2\Theta, \tag{101}$$

with solutions of the form:

$$\Theta = Ae^{\pm ic\theta}. \tag{102}$$

But θ is an angle, so we require periodic boundary conditions:

$$\Theta(\theta + 2\pi) = \Theta(\theta). \tag{103}$$

Hence $c = n$, an integer.

Thus, we have a differential equation in r only

$$\frac{r}{R}\frac{d}{dr}\left(r\frac{dR}{dr}\right) + r^2\nu^2 - n^2 = 0, \tag{104}$$

or

$$\frac{d}{dr}\left(r\frac{dR}{dr}\right)+r\nu^2R-\frac{n^2}{r}R=0, \tag{105}$$

It appears that it may be more sensible to regard n^2 as a given constant, and to treat ν^2 as the eigenvalue, related to k and the boundary conditions of the z equation. The equation is then in Sturm-Liouville form with:

$$\begin{aligned} p(r) &= r && (106)\\ q(r) &= n^2/r && (107)\\ w(r) &= r && (108)\\ \lambda &= \nu^2. && (109) \end{aligned}$$

Note that if we let $x=\nu r$ and $u=R$ we obtain the Bessel's equation, Eqn. 91, that we started with.

The solutions to Bessel's equation are denoted $J_n(x)=J_n(\nu r)$ and $Y_n(x)=Y_n(\nu r)$. The orthogonality condition for the J_n solutions reads:

$$\int_a^b J_n(\nu x)J_n(\mu x)xdx=\frac{x}{\nu^2-\mu^2}\left[\mu J_n(\nu x)J_n'(\mu x)-\nu J_n'(\nu x)J_n(\mu x)\right]_a^b. \tag{110}$$

This is 0 if $\nu\neq\mu$ and appropriate boundary conditions are specified. The normalization condition reads:

$$\int_a^b J_n^2(\nu x)dx=\frac{x^2}{2}\left[J_{n+1}(\nu x)\right]^2\Big|_a^b, \tag{111}$$

if the boundary condition $J_n(\nu a)=J_n(\nu b)=0$ is specified.

For example, suppose we wish to expand a function $f(x)$ on $[0,b]$:

$$f(x)=\sum_{m=1}^{\infty}c_mJ_n(k_nx), \tag{112}$$

where $J_n(k_nb)=0$. Then,

$$\int_a^b J_n(k_mx)J_n(k_px)xdx=\delta_{np}\frac{b^2}{2}\left[J_{n+1}(k_mb)\right]^2, \tag{113}$$

and

$$c_m=\frac{\int_0^b J_n(k_mx)f(x)xdx}{\frac{b^2}{2}\left[J_{n+1}(k_mb)\right]^2}. \tag{114}$$

4.4 Simple Harmonic Oscillator

The equation for the simple harmonic oscillator is:

$$\frac{d^2u}{dx^2} + \omega^2 u = 0. \tag{115}$$

This is already in Sturm-Liouville form, with

$$\begin{aligned} p(x) &= 1 && (116)\\ q(x) &= 0 && (117)\\ w(x) &= 1 && (118)\\ \lambda &= \omega^2. && (119) \end{aligned}$$

If $x \in [-a, a]$ with boundary condition $u(a) = u(-a) = 0$, the solutions are

$$u(x) = \sin\left(\pi n \frac{x}{a}\right), \tag{120}$$

with $\lambda_n = \omega^2 = (\pi n/a)^2$, and n is an integer.

4.5 Hermite Equation

The Schrödinger equation for the one-dimensional harmonic oscillator is

$$-\frac{d^2\psi}{dx^2} + x^2\psi = E\psi, \tag{121}$$

in units where $\hbar = 1$, mass $m = 1/2$, and spring constant $k = 2$. This is already essentially in Sturm-Liouville form.

However, we expect to satisfy boundary conditions $\psi(\pm\infty) = 0$. A useful approach, when we have such criteria, is to "divide out" the known behavior. For large x, $\psi(x) \to 0$, so in this regime the equation becomes, approximately:

$$\frac{d^2\psi}{dx^2} - x^2\psi = 0. \tag{122}$$

The solution, satisfying the boundary conditions, to this equation is $\psi(x) \sim \exp(-x^2/2)$. Thus, we'll let

$$\psi(x) = u(x)e^{-x^2/2}. \tag{123}$$

Substituting this form for $\psi(x)$ into the original Schrödinger equation yields the following differential equation for $u(x)$:

$$\frac{d^2u}{dx^2} - 2x\frac{du}{dx} + 2\alpha u = 0, \tag{124}$$

where we have set $E-1=2\alpha$. This is called the **Hermite Equation**.

From the way we obtained the Hermite equation, we have a clue for putting it into Sturm-Liouville form. If we let

$$p(x)=e^{-x^2}, \tag{125}$$

we have,

$$\frac{d}{dx}\left[p(x)\frac{du}{dx}\right]=e^{-x^2}\frac{d^2u}{dx^2}-2xe^{-x^2}\frac{du}{dx}. \tag{126}$$

Thus we have Sturm-Liouville form if we also let:

$$\begin{aligned} q(x) &= 0 \\ w(x) &= e^{-x^2} \\ \lambda &= 2\alpha. \end{aligned} \tag{127}$$

If we have $\alpha=n=0,1,2,\ldots$, then we have polynomial solutions called the Hermite polynomials, $H_n(x)$.

4.6 Laguerre Equation

The Laguerre Equation is:

$$x\frac{d^2u}{dx^2}+(1-x)\frac{du}{dx}+\alpha u=0. \tag{128}$$

It arises, for example, in the radial equation for the hydrogen atom Schrödinger equation. With a similar approach as that for the Hermite equation above, we can put it into Sturm-Liouville form with:

$$\begin{aligned} p(x) &= xe^{-x} \\ q(x) &= 0 \\ w(x) &= e^{-x} \\ \lambda &= \alpha. \end{aligned} \tag{129}$$

If we have $\alpha=n=0,1,2,\ldots$, then we have polynomial solutions called the Laguerre polynomials, $L_n(x)$:

$$L_n(x)=\frac{e^x}{n!}\frac{d^n}{dx^n}\left(x^n e^{-x}\right) \tag{130}$$

4.7 Associated Laguerre Equation

A modification to the Laguerre equation yields the associated Laguerre equation:

$$x\frac{d^2u}{dx^2} + (k+1-x)\frac{du}{dx} + (\alpha - k)u = 0, \tag{131}$$

where $k = 0, 1, 2, \ldots$. It may likewise be put into Sturm-Liouville form.

For $\alpha = n = 0, 1, 2, \ldots$ we have polynomial solutions:

$$L_n^k(x) = \frac{d^k}{dx^k}L_n(x), \tag{132}$$

although conventions differ. This equation, and the polynomial solutions arise also in the radial dependence of the hydrogen atom energy states with orbital angular momentum.

4.8 Hypergeometric Equation

The hypergeometric equation is:

$$x(1-x)u'' + [c - (a+b+1)x]\,u' - abu = 0. \tag{133}$$

This may be put into Sturm-Liouville form with:

$$\begin{aligned} p(x) &= \left(\frac{x}{1-x}\right)^c (1-x)^{a+b+1} \\ q(x) &= 0 \\ w(x) &= \frac{p(x)}{x(1-x)} \\ \lambda &= -ab. \end{aligned} \tag{134}$$

Mathews and Walker further discusses the hypergeometric equation and its partner the confluent hypergeometric equation, and the relation of the solutions to a variety of other special functions.

4.9 Chebyshev Equation

Beginning with the hypergeometric equation, let $a = -b = n$, where n is an integer. Also, let $c = 1/2$. Then the differential equation is:

$$x(1-x)u'' + \left[\frac{1}{2} - x\right]u'n^2u = 0. \tag{135}$$

If we further let $z = 1 - 2x$, this equation is transformed to:

$$(1 - z^2)\frac{d^2u}{dz^2} - z\frac{du}{dz} + n^2 u = 0. \tag{136}$$

This is called the Chebyshev differential equation (with a variety of spellings in the translation of the name).

This may be put into Sturm-Liouville form with:

$$\begin{aligned} p(z) &= \left(1 - z^2\right)^{1/2} \\ q(z) &= 0 \\ w(z) &= 1/p(z) \\ \lambda &= n^2. \end{aligned} \tag{137}$$

Solutions include the "Chebyshev polynomials of the first kind", $T_n(z)$. These polynomials have the feature that their oscillations are of uniform amplitude in the interval $[-1, 1]$.

5 Classical Orthogonal Polynomials

We find that a large class of our special functions can be described as "orthogonal polynomials" in the real variable x, with real coefficients:

Definition: A set of polynomials, $\{f_n(x) : n = 0, 1, 2, \ldots\}$, where f_n is of degree n, defined on $x \in [a, b]$ such that

$$\int_a^b f_n(x) f_m(x) w(x) dx = 0, \qquad n \neq m, \tag{138}$$

is called **orthogonal** on $[a, b]$ with respect to **weight** $w(x)$. We require that $w(x) \geq 0$.

5.1 General Properties of Orthogonal Polynomials

We may remark on some properties of orthogonal polynomials:

- The different systems of orthogonal polynomials are distinguished by the weight function and the interval. That is, the system of polynomials in $[a, b]$ is uniquely determined by $w(x)$ up to a constant for each polynomial. The reader may consider proving this by starting with the $n = 0$ polynomial and thinking in terms of the Gram-Schmidt algorithm.

- The choice of value for the remaining multiplicative constant for each polynomial is called **standardization**.
- After standardization, the normalization condition is written:

$$\int_a^b f_n(x)f_m(x)w(x)dx = h_n\delta_{nm}. \tag{139}$$

- The following notation is often used for the polynomials:

$$f_n(x) = k_n x^n + k_n' x^{n-1} + k_n'' x^{n-2} + \ldots + k^{(n)}, \tag{140}$$

  where $n = 0, 1, 2, \ldots$
- Note that with suitable weight function, infinite intervals are possible.

We'll discuss orthogonal polynomials here from an intuitive perspective. Start with the following theorem:

Theorem: The orthogonal polynomial $f_n(x)$ has n real, simple zeros, all in (a, b) (note that this excludes the boundary points).

Let us argue the plausibility of this. First, we notice that since a polynomial of degree n has n roots, there can be no more than n real, simple zeros in (a, b). Second, we keep in mind that $f_n(x)$ is a continuous function, and that $w(x) \geq 0$.

Then we may adopt an inductive approach. For $n = 0$, $f_0(x)$ is just a constant. There are zero roots, in agreement with our theorem. For $n > 0$, we must have

$$\int_a^b f_n(x)f_0(x)w(x)dx = 0. \tag{141}$$

If f_n nowhere goes through zero in (a, b), we cannot accomplish this. Hence, there exists at least one real root for each f_n with $n > 0$.

For $n = 1$, $f_1(x) = \alpha + \beta x$, a straight line. It must go through zero somewhere in (a, b) as we have just argued, and a straight line can have only one zero. Thus, for $n = 1$ there is one real, simple root.

For $n > 1$, consider the possiblities: We must have at least one root in (a, b). Can we accomplish orthogonality with exactly two degenerate roots? Certainly not, because then we cannot be orthogonal with f_0 (the polynomial will always be non-negative or always non-positive in (a, b)). Can we be orthogonal to both f_0 and f_1 with only one root? By considering the possibilities for where this root could be compared with the root of f_1, and imposing orthogonality with f_0, it may be readily seen that this doesn't work either.

The reader is invited to develop this into a rigorous proof. Thus, there must be at least two distinct real roots in (a, b) for $n > 1$. For $n = 2$, there are thus exactly two real, simple roots in (a, b).

The inductive proof would then assert the theorem for all $k < n$, and demonstrate it for n.

Once we are used to this theorem, the following one also becomes plausible:

Theorem: The zeros of $f_n(x)$ and $f_{n+1}(x)$ alternate (and do not coincide) on (a, b).

These two theorems are immensely useful for qualtitative understanding of solutions to problems, without ever solving for the polynomials. For example, the qualitative nature of the wave functions for the different energy states in a quantum mechanical problem may be pictured.

The following theorem is also intuitively plausible:

Theorem: For any given subinterval of (a, b) there exists an N such that whenever $n > N$, $f_n(x)$ vanishes at least once in the subinterval. That is, the zeros of $\{f_n(x)\}$ are dense in (a, b).

Note the plausibility: The alternative would be that the zeros somehow decided to "bunch up" at particular places. But this would then make satisfying the orthogonality difficult (impossible).

Finally, we have the "approximation" theorem:

Theorem: Given an arbitrary function $g(x)$, and all polynomials $\{p_k : k \leq n\}$ of degree less than or equal to n (linear combinations of $\{f_k\}$), there exists exactly one polynomial q_n for which $|g - q_n|$ is minimized:

$$q_n(x) = \sum_{k=0}^{n} a_k f_k(x), \tag{142}$$

where

$$a_k = \frac{\langle f_k | g \rangle}{h_k}. \tag{143}$$

If $g(x)$ is continuous, then $g(x) - q_n(x)$ changes sign at least $n+1$ times in (a, b), or else vanishes identically.

This theorem asserts that any polynomial of degree less than or equal to n can be expressed as a linear combination of the orthogonal polynomials of degree $\leq n$. This is clearly possible, as an explicit construction along the lines of Eqs. 142 and 143 can be performed.

The plausiblity of the remainder of the theorem may be seen by first noticing that

$$\sum_{k=0}^{n} \frac{|f_k\rangle\langle f_k|g\rangle}{h_k} \tag{144}$$

projects out the component of g in the subspace spanned by $f_0, f_1, \ldots, f_n$. Any component of g which is orthogonal to this subspace is unreachable, the best we can do is perfectly approximate the component in the subspace. That is, write $g = g_{\parallel} + g_{\perp}$, as the decomposition into the components of g within and orthognonal to the subspace spanned by $\{f_k, k = 1, 2, \ldots, n\}$. We'll take $h_k = 1$ for simplicity here. By definition,

$$\langle g_{\perp}|f_k\rangle = 0, \quad k = 0, 1, 2, \ldots, n, \tag{145}$$

and we expect that

$$g_{\parallel} = \sum_{k=0}^{n} a_k f_k = q_n. \tag{146}$$

Then we see that

$$\begin{aligned} |g - q_n|^2 &= \langle g_{\parallel} + g_{\perp} - q_n | g_{\parallel} + g_{\perp} - q_n\rangle \\ &= \langle g_{\parallel} - q_n | g_{\parallel} - q_n\rangle + \langle g_{\perp}|g_{\perp}\rangle \\ &= \langle g_{\perp}|g_{\perp}\rangle \end{aligned} \tag{147}$$

But since, by the triangle inequality, for any vector u

$$|g - u|^2 \leq |g_{\parallel} - u|^2 + |g_{\perp}|^2. \tag{148}$$

Hence we have done the best we can with a function which is orthogonal to $g_{\perp}$.

5.2 Generalized Rodrigues' Formula

The **Rodrigues' formula** for the Legendre polynomials is:

$$P_n(x) = \frac{(-1)^n}{2^n n!} \frac{d^n}{dx^n} \left(1 - x^2\right)^n. \tag{149}$$

This form may be generalized to include some of the other systems of polynomials, obtaining the **generalized Rodrigues' formula**:

$$f_n(x) = \frac{1}{K_n w(x)} \frac{d^n}{dx^n} \left\{w(x) \left[s(x)\right]^n\right\}, \tag{150}$$

where K_n is the "standardization" and $s(x)$ is a polynomial (generally of degree 2), independent of n. We remark that not all possible weight functions will produce polynomials with this equation. For the Legendre polynomials, $w(x) = 1$ and the normalization is:

$$\int_{-1}^{1} [P_\ell(x)]^2 \, dx = \frac{2}{2\ell + 1}. \tag{151}$$

Corresponding to the generalized Rodrigues' formula, we have the Sturm-Liouville equation for orthogonal polynomials:

$$\frac{d}{dx}\left[s(x)w(x)\frac{df_n}{dx}(x)\right] + w(x)\lambda_n f_n(x) = 0, \tag{152}$$

where

$$\lambda_n = -n\left[K_1\frac{df_1}{dx} + \frac{1}{2}(n-1)\frac{d^2 s}{dx^2}\right]. \tag{153}$$

5.3 Recurrence Relation

The recurrence relation for the orthogonal polynomials may be expressed in the form:

$$f_{n+1}(x) = (a_n + b_n x)\, f_n(x) - c_n f_{n-1}(x), \tag{154}$$

where

$$b_n = \frac{k_{n+1}}{k_n} \tag{155}$$

$$a_n = b_n\left(\frac{k'_{n+1}}{k_{n+1}} - \frac{k'_n}{k_n}\right) \tag{156}$$

$$c_n = \frac{h_n}{h_{n-1}}\frac{k_{n+1}k_{n-1}}{k_n^2}, \tag{157}$$

and $c_0 = 0$. The k_n notation here is that of Eqn. 140.

We may define the following "projection operator", onto the subspace spanned by the first $n+1$ orthogonal polynomials:

$$J_n(x,y) \equiv \sum_{j=0}^{n} \frac{f_j(x)f_j(y)}{h_j}. \tag{158}$$

We then have the following theorem:

Theorem:

$$J_n(x,y) = \frac{k_n}{h_n k_{n+1}}\frac{f_n(y)f_{n+1}(x) - f_{n+1}(y)f_n(x)}{x-y}. \tag{159}$$

This is known as the **Christoffel-Darboux theorem**.

Let us prove this theorem: Multiply both sides by $(x-y)$ and evaluate between $\langle f_i|$ and $|f_k\rangle$. The right side gives:

$$\begin{aligned}
\frac{k_n}{h_n k_{n+1}}\left(\langle f_i|f_n\rangle\langle f_{n+1}|f_k\rangle - \langle f_i|f_{n+1}\rangle\langle f_n|f_k\rangle\right) &= \frac{k_n}{h_n k_{n+1}}\left(\delta_{in}\delta_{(n+1)k} - \delta_{i(n+1)}\delta_{nk}\right) \\
&= \frac{k_n}{h_n k_{n+1}}\begin{cases} 0 & i=k \\ 1 & i=n \text{ and } k=n+1 \\ -1 & i=n+1 \text{ and } k=n \\ 0 & \text{otherwise.}\end{cases} \qquad (160)
\end{aligned}$$

The other side evalutes to:

$$\begin{aligned}
\langle f_i|(x-y)\sum_{j=0}^{n}\frac{1}{h_j}f_j(x)f_j(y)|f_k\rangle &= \sum_{j=0}^{n}\frac{1}{h_j}\left(\langle f_i|f_j\rangle\langle xf_j|f_k\rangle - \langle f_i|yf_j\rangle\langle f_j|f_k\rangle\right) \\
&= \sum_{j=0}^{n}\frac{1}{h_j}\left(\delta_{ij}\langle xf_j|f_k\rangle - \delta_{kj}\langle f_i|xf_j\rangle\right) \\
&= \begin{cases} 0 & i>n \text{ and } k>n \\ 0 & i\le n \text{ and } k\le n \\ \langle xf_i|f_k\rangle/h_i & i\le n \text{ and } k>n \\ -\langle f_i|xf_k\rangle/h_k & i>n \text{ and } k\le n.\end{cases} \qquad (161)
\end{aligned}$$

Thus, we must evaluate, for example, $\langle f_i|xf_k\rangle$. We use the recurrence relation:

$$f_{k+1} = (a_k + b_k x)f_k - c_k f_{k-1}, \qquad (162)$$

or,

$$xf_k = \frac{1}{b_k}\left(f_{k+1} - a_k f_k + c_k f_{k-1}\right). \qquad (163)$$

Therefore,

$$\begin{aligned}
\langle f_i|xf_k\rangle &= \frac{1}{b_k}\left(\langle f_i|f_{k+1}\rangle - a_k\langle f_i|f_k\rangle + c_k\langle f_i|f_{k-1}\rangle\right) \\
&= \frac{1}{b_k}\left(\delta_{i(k+1)} - a_k\delta_{ik} + c_k\delta_{i(k-1)}\right). \qquad (164)
\end{aligned}$$

In this case, the only possibility we need concern ourselves with is $i=n+1$ and $k=n$. Then

$$\begin{aligned}
\langle f_i|xf_k\rangle &= \frac{1}{b_n} \\
&= \frac{k_n}{k_{n+1}}, \qquad (165)
\end{aligned}$$

which is the desired result. A similar analysis is obtained for the $\langle xf_i|f_k\rangle$ case, with $i\le n$ and $k>n$.

Note that the Christoffel-Darboux formula accomplishes the translation of an operator which projects onto the subspace spanned by the first $n+1$ polynomials into the form of a simple, symmetric kernel.

5.4 Example: Hermite Polynomials

The Hermite polynomials, $H_n(x)$, satisfy the differential equation:

$$\frac{d^2}{dx^2}H_n(x) - 2x\frac{d}{dx}H_n(x) + 2nH_n(x) = 0, \tag{166}$$

where $x \in [a,b] = [-\infty, \infty]$. We can put this into Sturm-Liouville form with:

$$\begin{aligned} p(x) &= e^{-x^2} \qquad (167) \\ q(x) &= 0 \\ w(x) &= e^{-x^2} \qquad (168) \\ \lambda &= 2n. \end{aligned}$$

This gives:

$$\frac{d}{dx}\left(e^{-x^2}\frac{dH_n}{dx}\right) + 2ne^{-x^2}H_n(x) = 0, \tag{169}$$

To obtain the generalized Rodrigues' formula for the Hermite polynomials, we note that since $p(x) = s(x)w(x)$, we must have $s(x) = 1$. Hence, the generalized Rodrigues' formula is:

$$\begin{aligned} H_n(x) &= \frac{1}{K_n w(x)}\frac{d^n}{dx^n}\left[w(x)s(x)^n\right] \\ &= \frac{e^{x^2}}{K_n}\frac{d^n}{dx^n}e^{-x^2}. \qquad (170) \end{aligned}$$

Since

$$\frac{d}{dx}e^{-x^2} = -2xe^{-x^2}, \tag{171}$$

the order x^n leading term is

$$e^{x^2}\frac{d^n}{dx^n}e^{-x^2} = (-2)^n x^n + O(x^{n-1}). \tag{172}$$

Hence $k_n = 2^n$. The reader may demonstrate that $k_n' = 0$, and also that the normalization is

$$h_n = \sqrt{\pi}2^n n!. \tag{173}$$

6 Green's Function for the Inhomogeneous Sturm-Liouville Equation

We now give a general discussion of the problem of obtaining the Green's function for the inhomogeneuos Sturm-Liouville problem. The problem is to find u satisfying:

$$Lu = (pu')' - qu = -\phi, \tag{174}$$

for $x \in [a, b]$, and where $\phi(x)$ is a continuous function of x. We look for a solution in the form of the integral equation:

$$u(x) = \int_a^b G(x, y)\phi(y)dy. \tag{175}$$

Thus, we wish to find $G(x, y)$.

We make some intitial observations to guide our determination of G:

1. Since $u(x)$ satisfies the boundary conditions, $G(x, y)$ must also, at least in x.

2. Presuming p and q are continuous functions, $G(x, y)$ is a continuous function of x.

3. $G' \equiv \frac{\partial G(x,y)}{\partial x}$ and G'' are continuous functions of x, except at $x = y$, where
$$\lim_{\epsilon \to 0} [G'(y + \epsilon, y) - G'(y - \epsilon, y)] = -\frac{1}{p(y)}. \tag{176}$$

4. Except at $x = y$, G satisfies the differential equation $L_x G = 0$.

We remark that properties 2-4 follow from the operator equation:

$$L_x G(x, y) = -\delta(x - y), \tag{177}$$

where the minus sign here is from the $-\phi$ on the right hand side of Eqn. 174. Writing this out:

$$L_x G = pG'' + p'G' - qG = -\delta(x - y). \tag{178}$$

The second derivative term must be the term that gives the delta function. That is, in the limit as $\epsilon \to 0$:

$$\int_{y-\epsilon}^{y+\epsilon} p(x)G''(x, y)dx = -1. \tag{179}$$

But $p(x)$ is continuous, hence can be evaluated at $x = y$ and removed from the integral in this limit, yielding

$$\int_{y-\epsilon}^{y+\epsilon} G''(x,y)dx = -\frac{1}{p(y)}. \tag{180}$$

Integrating, we obtain the result asserted in Eqn. 176.

As we have remarked before, there are various approaches to finding G. Here, we'll attempt to find an explicit solution to $L_x G(x,y) = -\delta(x-y)$.

Suppose that we have found two linearly independent solutions $u_1(x)$ and $u_2(x)$ to the homogeneous equation $Lu = 0$, without imposing the boundary conditions. It may be noted here that a sufficient condition for independence of two solutions to be independent is that the Wronskian not vanish. Here, the Wronskian is:

$$W(x) = u_1(x)u_2'(x) - u_1'(x)u_2(x). \tag{181}$$

The conditon for independence is that u_1 and u_2 are linearly independent if $k_1 u_1 + k_2 u_2 = 0$ implies $k_1 = k_2 = 0$. Consider the derivative of this:

$$k_1 u_1' + k_2 u_2' = 0. \tag{182}$$

Inserting $k_2 = -k_1 u_1/u_2$, we obtain

$$k_1 \left(u_1' u_2 - u_1 u_2'\right) = -k_1 w(x) = 0. \tag{183}$$

Thus, either $k_1 = k_2 = 0$ or the Wronskian vanishes. If the Wronskian does not vanish, then the two solutions are linearly independent.

In some cases, the Wronskian is independent of x; consider the derivative:

$$W'(x) = u_1(x)u_2''(x) - u_1''(x)u_2(x). \tag{184}$$

With $Lu_j = 0$, we have

$$p(x)u_j''(x) + p'(x)u_j'(x) - q(x)u_j(x) = 0. \tag{185}$$

Thus,

$$u_j''(x) = \frac{q(x)}{p(x)}u_j(x) - \frac{p'(x)}{p(x)}u_j'(x). \tag{186}$$

Hence,

$$\begin{aligned} W'(x) &= -\frac{p'(x)}{p(x)}\left[u_1(x)u_2'(x) - u_1'(x)u_2(x)\right] \\ &= -\frac{p'(x)}{p(x)}W(x). \end{aligned} \tag{187}$$

This is zero if $p' = 0$, that is if $p(x)$ is a constant function, and hence if there is no first order derivative in the differential equation. When this is true, it is very convenient, since it means that the Wronskian can be evaluated at any convenient point.

With two linearly independent solutions, the general solution to $Lu = 0$ is

$$u = c_1 u_1 + c_2 u_2. \tag{188}$$

Since $G(x, y)$ satisfies the homogeneous differential equation $L_x G = 0$ except at $x = y$, we may form a "right" and a "left" solution:

$$G(x, y) = \begin{cases} (A - \alpha)u_1(x) + (B - \beta)u_2(x), & x \leq y, \\ (A + \alpha)u_1(x) + (B + \beta)u_2(x), & x \geq y. \end{cases} \tag{189}$$

The four "constants" A, B, α, β, which may depend on y, have been chosen in this way for following convenience. Note that $x = y$ has been included for the two solutions, since G must be continuous.

Imposing continuity at $x = y$:

$$(A - \alpha)u_1(y) + (B - \beta)u_2(y) = (A + \alpha)u_1(y) + (B + \beta)u_2(y). \tag{190}$$

This yields

$$\alpha u_1(y) + \beta u_2(y) = 0. \tag{191}$$

The derivative has a discontinuity at $x = y$:

$$\begin{aligned} \frac{1}{p(y)} &= G'(y - \epsilon, y) - G'(y + \epsilon, y) \\ &= (A - \alpha)u_1'(y) + (B - \beta)u_2' - (A + \alpha)u_1'(y) + (B + \beta)u_2'(y) \\ &= -2\left[\alpha u_1'(y) + \beta u_2'(y)\right]. \end{aligned} \tag{192}$$

We thus have two equations in the unknowns α and β. Solving, we obtain:

$$\alpha(y) = \frac{u_2(y)}{2p(y)W(y)} \tag{193}$$

$$\beta(y) = -\frac{u_1(y)}{2p(y)W(y)}. \tag{194}$$

We thus have the Green's function for the Sturm-Liouville operator:

$$G(x, y) = A(y)u_1(x) + B(y)u_2(x) + \begin{pmatrix} - \\ + \end{pmatrix} \frac{u_1(x)u_2(y) - u_2(x)u_1(y)}{2p(y)W(y)} \quad \begin{matrix} x \leq y \\ x \geq y \end{matrix}. \tag{195}$$

By construction, this satisfies $L_x G(x,y) = -\delta(x-y)$. The "constants" A and B are to be determined by the boundary conditions of the specific problem. The solution to the inhomogeneous equation $Lu = -\phi$ is:

$$u(x) = \int_a^b G(x,y)\phi(y)dy. \tag{196}$$

We remark again that the Green's function for a self-adjoint operator (as in the Sturm-Liouville problem with appropriate boundary conditions) is symmetric, and thus the Schmidt-Hilbert theory applies.

It may happen, however, that we encounter boundary conditions such that we cannot find A and B to satisfy them. In this case, we may attempt to find an appropriate "modified" Green's fucntion as follows: Suppose that we can find a solution u_0 to $Lu_0 = 0$ that satisfies the boundary conditions (that is, suppose there exists a solution to the homogeneous equation). Let's suppose here that the specified boundary conditions are homogeneous. Then cu_0 is also a solution, and we may assume that u_o has been normalized:

$$\int_a^b [u_0(x)]^2 \, dx = 1. \tag{197}$$

Now find a Green's function which satisfies all the same properties as before, except that now:

$$LG(x,y) = u_0(x)u_0(y), \qquad \text{for } x \neq y, \tag{198}$$

and

$$\int_a^b G(x,y)u_0(x)dx = 0. \tag{199}$$

The resulting Green's function will still be symmetric, and the solution to our problem is still

$$u(x) = \int_a^b G(x,y)\phi(y)dy. \tag{200}$$

Let us try it:

$$\begin{aligned} Lu &= \int_a^b L_x G(x,y)\phi(y)dy \\ &= \int_a^b \left[-\delta(x-y)\right]\phi(y)dy + \int_a^b u_0(x)u_0(y)\phi(y)dy \\ &= -\phi(x) + u_0(x)\int_a^b u_0(y)\phi(y)dy. \end{aligned} \tag{201}$$

This works if $\int_a^b u_0(y)\phi(y)dy = 0$, that is if ϕ and u_0 are orthogonal. If this doesn't hold, then there is no solution to the problem which satisfies the boundary conditions.

6.1 Example

Let's try an example to illustrate these ideas. Consider $Lu = u'' = -\phi(x)$, plus interval and boundary conditions to be specified. Find the Green's function: Two solutions to $Lu = 0$ are:

$$u_1(x) = 1, u_2(x) = x. \tag{202}$$

Note that $p(x) = 1$. The Wronskian will be a constant in this case, so evaluate it at $x = 0$ (this really doesn't save any work in this simple example, but we do it anyway for illustration):

$$W(x) = u_1(0)u_2'(0) - u_1'(0)u_2(0) = 1. \tag{203}$$

Using equation 195, we have:

$$\begin{aligned} G(x,y) &= A(y) + B(y)x + \frac{\mp 1}{2}\left[u_1(x)u_2(y) - u_2(x)u_1(y)\right] \quad \begin{matrix} x \le y \\ x \ge y \end{matrix} \\ &= A(y) + B(y)x + \frac{\mp 1}{2}(y - x) \quad \begin{matrix} x \le y \\ x \ge y. \end{matrix} \end{aligned} \tag{204}$$

Now suppose that the range of interest is $x \in [-1, 1]$. Let the boundary conditions be periodic:

$$u(1) = u(-1) \tag{205}$$

$$u'(1) = u'(-1). \tag{206}$$

To satisfy $G(1, y) = G(-1, y)$ we must have:

$$A + B + \frac{1}{2}(y - 1) = A - B - \frac{1}{2}(y + 1). \tag{207}$$

This is satisfied if $B = -y/2$, and we have:

$$G(x,y) = A(y) - \frac{xy}{2} + \frac{\mp 1}{2}(y - x) \quad \begin{matrix} x \le y \\ x \ge y. \end{matrix} \tag{208}$$

For the other boundary condition, take:

$$\begin{aligned} \frac{\partial G}{\partial x}(x,y) &= -\frac{y}{2} \mp \left(-\frac{1}{2}\right) \quad \begin{matrix} x \le y \\ x \ge y. \end{matrix} \\ &= -\frac{1}{2}\left(y \mp 1\right) \quad \begin{matrix} x \le y \\ x \ge y. \end{matrix} . \end{aligned} \tag{209}$$

Thus, $G'(1, y) = -\frac{1}{2}(y + 1) \neq G'(-1, y) = -\frac{1}{2}(y - 1)$; the periodic boundary condition in the derivative cannot be satisfied.

We turn to the modified Green's function in hopes of rescuing the situation. We want to find a solution, u_0, to $Lu_0 = 0$ which satisfies the boundary conditions and is normalized:

$$\int_{-1}^{1} u_0^2(x)dx = 1. \tag{210}$$

The solution $u_0 = 1/\sqrt{2}$ satisfies all of these conditions. We modify our Green's function so that

$$L_x G(x,y) = \frac{\partial^2}{\partial x^2} G(x,y) = u_0(x)u_0(y) = \frac{1}{2}, \quad x \neq y. \tag{211}$$

This is accomplished by adding $x^2/4$ to our unmodified Green's function:

$$G(x,y) = A(y) - \frac{xy}{2} + \frac{x^2}{4} + \begin{matrix} - \\ + \end{matrix} \frac{1}{2}(y-x) \quad \begin{matrix} x \leq y \\ x \geq y. \end{matrix} \tag{212}$$

Note that our condition on B remains the same as before, since the added $x^2/4$ term separately satisfies the $u(-1) = u(1)$ boundary condition.

The boundary condition on the derivative involves

$$G'(x,y) = -\frac{y}{2} + \frac{x}{2} + \begin{matrix} - \\ + \end{matrix} \left(-\frac{1}{2}\right) \quad \begin{matrix} x \leq y \\ x \geq y. \end{matrix} \tag{213}$$

We find that

$$G'(1,y) = -\frac{y}{2} = G'(-1,y). \tag{214}$$

Finally, we fix A by requiring

$$\int_a^b G(x,y)u_0(x)dx = 0. \tag{215}$$

Substituting in,

$$\int_{-1}^{1} \left(A - \frac{xy}{2} + \frac{x^2}{4}\right) dx + \int_{-1}^{y} \frac{x-y}{2} dx - \int_{y}^{1} \frac{x-y}{2} dx = 0. \tag{216}$$

Solving for A gives:

$$A = \frac{1}{6} + \frac{y^2}{4}. \tag{217}$$

Thus,

$$G(x,y) = \frac{1}{6} + \frac{1}{4}(x-y)^2 + \begin{matrix} - \\ + \end{matrix} \frac{1}{2}(y-x) \quad \begin{matrix} x \leq y \\ x \geq y. \end{matrix} \tag{218}$$

This may alternatively be written

$$G(x,y) = \frac{1}{6} + \frac{1}{4}(x-y)^2 + \left[\frac{1}{2} - \theta(x-y)\right](x-y). \tag{219}$$

Note that the Green's function is symmetric, $G(x,y) = G(y,x)$.

Now let us suppose that $\phi(x) = -1$. But our procedure for choosing A implies that in this case,

$$u(x) = \int_{-1}^{1} G(x,y)\phi(y)dy = 0. \tag{220}$$

No solution exists for $\phi(y) = -1$. Notice that

$$\int_{-1}^{1} \phi(x)u_0(x)dx = -\frac{1}{\sqrt{2}}\int_{-1}^{1} dx \neq 0. \tag{221}$$

This problem is sufficiently simple that the reader is encouraged to demonstrate the non-existence of a solution by elementary methods.

Let us suppose, instead, that $\phi(x) = x$, that is we wish to solve $Lu = -x$. Note that

$$\int_{-1}^{1} \phi(x)u_0(x)dx = \frac{1}{\sqrt{2}}\int_{-1}^{1} xdx = 0, \tag{222}$$

so now we expect that a solution will exist. Let's find it:

$$\begin{aligned} u(x) &= \int_{-1}^{1} G(x,y)\phi(y)dy \\ &= \frac{1}{6}\int_{-1}^{1} ydy + \frac{1}{4}\int_{-1}^{1}(x-y)^2 ydy + \frac{1}{2}\int_{-1}^{x}(y-x)ydy - \frac{1}{2}\int_{x}^{1}(y-x)ydy \\ &= -\frac{x^3}{6} + \frac{x}{6} + \text{arbitrary constant } C. \end{aligned} \tag{223}$$

We added the arbitrary constant, because any multiple of u_0, the solution to the homogeneous equation (including boundary conditions) can be added to the solution to obtain another solution. Our solution is thus not unique.

6.2 Green's Function Wrap-up

Let us try to understand what is happening in the example we have just investigated, in the context of our more general discussion. Recall from the alternative theorem that when a solution to the homogeneous equation (with homogeneous boundary conditions) exists, the solution to the inhomogeneous equation either does not exist, or is not unique. A solution exists if and only if ϕ is perpendicular to any solution of the homogeneous equation, e.g.,

$$\int_a^b \phi(x)u_0(x)dx = 0. \tag{224}$$

We examine this further in the context of an expansion in eigenfunctions. When we considered the problem $Lu = g$, we obtained the expansion:

$$G = \sum_i \frac{|u_i\rangle\langle u_i|}{\lambda_i}. \tag{225}$$

But u_0 is a non-trivial solution which corresponds to eigenvalue $\lambda_0 = 0$. The expansion above doesn't work in this case. However, we also considered the problem $Lu - \lambda u = g$, and the expansion:

$$G = \sum_i \frac{|u_i\rangle\langle u_i|}{\lambda_i - \lambda}. \tag{226}$$

This now works fine for u_0 as long as $\lambda \neq 0$, and we can solve $Lu = -\phi$ as long as $\langle u_0|\phi\rangle = 0$ (so that taking the $\lambda \to 0$ limit will not cause trouble). But then any constant times u_0 will also be a solution.

For our explicit approach to finding the Green's function we are led to consider a source term, or "force" in $LG =$ "source(x, y)" that contains not only the $\delta(x - y)$ point source, but an additional source that prevents the homogeneous solution from blowing up – note that $\delta(x-y)$ is not orthogonal to u_0. We add a "restoring force" to counteract the presence of a u_0 piece in the δ term.

There is some arbitrariness to this additional source, but it cannot be orthogonal to the eigenfunction u_0 if it is to prevent the "excitation" of this mode by the δ source. Thus, the usual choice, with nice symmetry, is

$$L_xG(x, y) = -\delta(x - y) + u_0(x)u_0(y). \tag{227}$$

Note that:

$$\int_a^b [-\delta(x - y) + u_0(x)u_0(y)]\, u_0(y)dy = -u_0(x) + u_0(x) = 0, \tag{228}$$

since we have $\langle u_0|u_0\rangle = 1$. The additional term exactly cancels the u_0 "component" of the δ source.

Since $Lu_0 = 0$, this equation, including the boundary conditions, and the discontinuity condition on G' only determines $G(x, y)$ up to the addition of an arbitrary term $A(y)u_0(x)$. To pick out a particular function, we impose the requirement

$$\int_a^b G(x,y)u_o(x)dx = 0. \tag{229}$$

This particular requirement is chosen to yield a symmetric Green's function. To see why this works, consider:

$$L_x \int_a^b G(x,y)u_0(y)dy = \int_a^b \left[-\delta(x-y) + u_0(x)u_0(y)\right] u_0(y)dy = 0. \tag{230}$$

Thus, $\int_a^b G(x,y)u_0(y)dy$ is a function which satisfies $Lu = 0$, and satisfies the boundary conditions. But the most general such function (we're considering only second order differential equations here) is $cu_0(x)$, hence

$$\int_a^b G(x,y)u_0(y)dy = cu_0(x). \tag{231}$$

This implies that the solution to $Lu = -u_0$ is cu_0. But we know that $L(cu_0) = 0$, so there is no solution to $Lu = -u_0$. The only way to reconcile this with Eqn. 231 is with $c = 0$. That is, the integral on the left is well-defined, but it cannot be a non-trivial multiple of $u_0(x)$ because this would imply that the solution to $Lu = -u_0$ exists. Hence, the only possible value for the integral is zero:

$$\int_a^b G(x,y)u_0(y)dy = 0. \tag{232}$$

For symmetry, we thus also require:

$$\int_a^b G(x,y)u_0(x)dx = 0. \tag{233}$$

This additional requirement leads to a unique result for $Lu = -\phi$, as we saw in our example, but it must be remembered that the requirement is really arbitrary, since we can add any multiple of u_0 to our solution and obtain another solution.

We'll conclude with some further comments about the Sturm-Liouville problem.

1. Recall that our expression for $G(x,y)$ had a factor of $1/p(y)W(y)$ in the

$$\frac{u_1(x)u_2(y) - u_1(y)u_2(x)}{2p(y)W(y)} \tag{234}$$

term. Let's look at this factor, by taking the derivative:

$$\begin{aligned}
\frac{d}{dx}pW &= pW' + p'W \\
&= pu_1u_2'' - pu_1''u_2 + p'u_1u_2' - p'u_1'u_2 \\
&= u_1\left(pu_2'' + p'u_2'\right) - u_2\left(pu_1'' + p'u_1'\right) \\
&= u_1qu_2 - u_2qu_1 = 0.
\end{aligned} \tag{235}$$

Thus, $p(x)W(x)$ is independent of x, and the evaluation of the denominator may be made at at any convenient point, not only at $x = y$. This can be very useful when the identity yielding the constant isn't so obvious.

2. Let's quickly consider the complication of the weight function. Suppose

$$\phi(x) = \lambda w(x)u(x) - \psi(x), \tag{236}$$

corresponding to

$$Lu + \lambda wu = \psi. \tag{237}$$

Then we have

$$\begin{aligned}
u(x) &= \int_a^b G(x,y)\phi(y)dy \\
&= g(x) + \lambda\int_a^b G(x,y)w(y)u(y)dy,
\end{aligned} \tag{238}$$

where

$$g(x) = -\int_a^b G(x,y)\psi(y)dy. \tag{239}$$

This is familiar, except that if $w(y) \neq 1$ we no longer have a symmetric kernel. We can "fix" this by defining a new unknown function, $f(x)$ by

$$f(x) = u(x)\sqrt{w(x)}, \tag{240}$$

which is all right, since $w(x) \geq 0$. Substituting this into Eqn. 238, including multiplication of the equation by $\sqrt{w(x)}$, we have:

$$f(x) = \sqrt{w(x)}g(x) + \lambda\int_a^b \sqrt{w(x)}G(x,y)\sqrt{w(y)}f(y)dy. \tag{241}$$

The kernel $\sqrt{w(x)}G(x,y)\sqrt{w(y)}$ is now symmetric.

3. In some of the discussion above, we assumed homogeneous boundary conditions. Let us consider with an example the treatment of inhomogeneous boundary conditions. Suppose that we have the homogeneous differential equation $Lu = 0$, with $L = \frac{d}{dx}p(x)\frac{d}{dx} - q(x)$, with the inhomogeneous boundary conditions $u(0) = 0$ and $u(1) = 1$.

   We can transform this to an inhomogeneous problem with homogeneous boundary conditions: Let

$$v(x) = u(x) - x. \tag{242}$$

   Now the boundary conditions in $v(x)$ are homogeneous: $v(0) = v(1) = 0$. The differential equation becomes:

$$Lu = \frac{d}{dx}p(x)\frac{d}{dx}u(x) - q(x)u(x) = \frac{d}{dx}p(x)\frac{d}{dx}\left[v(x) + x\right] - q(x)v(x) - q(x)x = 0, \tag{243}$$

   or $Lv = -\phi$, where

$$\phi(x) = \frac{dp}{dx}(x) - q(x)x. \tag{244}$$

   Thus, we now have an inhomogeneous Sturm-Liouville problem with homogeneous boundary conditions. Note that we could just as well have picked $v(x) = u(x) - x^2$, or $v(x) = u(x) - \sin(\pi x/2)$. The possibilities are endless, one should try to pick something that looks like it is going to make the problem easy.

7 Green's Functions Beyond Sturm-Liouville

We have concentrated our discussion on the Sturm-Liouville problem, largely because so many real problems are of this form. However, the Green's function method isn't limited to solving this problem. We briefly remark on other applications here.

For a linear differential equation of order n, we can also look for a Green's function solution, with the properties:

$$LG(x, y) = -\delta(x - y), \tag{245}$$

or

$$\frac{\partial^n}{\partial x^n}G(x, y) + a_1(x)\frac{\partial^{n-1}}{\partial x^{n-1}}G(x, y) + \cdots + a_n(x)G(x, y) = -\delta(x - y). \tag{246}$$

Then $G(x,y)$ is a solution to the homogeneous equation except at $x = y$. At $x = y$, $G(x,y)$ and its first $n-2$ derivatives are continuous, but the $n-1$ derivative has a discontinuity of magnitude one:

$$\lim_{\epsilon\to 0}\left[\left(\frac{\partial^{n-1}G}{\partial x^{n-1}}\right)(y+\epsilon,y) - \left(\frac{\partial^{n-1}G}{\partial x^{n-1}}\right)(y-\epsilon,y)\right] = -1. \tag{247}$$

This will give the $-\delta(x-y)$ when the nth derivative is taken.

Note that for a differential equation of order greater than two, it may happen that there is more than one independent eigenvector associated with eigenvalue zero. In this case, we form the modified Green's function as follows: Suppose that $u_0(x), u_1(x), \ldots u_m(x)$ are the orthonormal eigenfunctions corresponding to $\lambda = 0$ (and satisfying the boundary conditions). Require that

$$L_x G(x,y) = \sum_{i=0}^{m} u_i(x)u_i(y), \quad x \neq y. \tag{248}$$

For symmetry, also require that

$$\int_a^b G(x,y)u_i(x)dx = 0, \quad i = 0,1,2,\ldots,m. \tag{249}$$

If a soluton to the inhomogeneous equation $Lu = -\phi$ exists, we must have

$$\int_a^b u_i(x)\phi(x)dx = 0, \quad i = 0,1,2,\ldots,m. \tag{250}$$

We finally remark that partial differential equations, involving more than one dimension may also be treated. The reader may wish to consult Courant and Hilbert for some of the subtleties in this case.

8 Exercises

1. Consider the general linear second order homogeneous differential equation in one dimemsion:

$$a(x)\frac{d^2}{dx^2}u(x) + b(x)\frac{d}{dx}u(x) + c(x)u(x) = 0. \tag{251}$$

Determine the conditions under which this may be written in the form of a differential equation involving a self-adjoint (with appropriate boundary conditions) **Sturm-Liouville operator**:

$$Lu = 0, \tag{252}$$

where

$$L = \frac{d}{dx}p(x)\frac{d}{dx} - q(x). \tag{253}$$

Note that part of the problem is to investigate self-adjointness.

2. Show that the operator

$$L = \frac{d^2}{dx^2} + 1, \quad x \in [0, \pi], \tag{254}$$

with homogeneous boundary conditions $u(0) = u(\pi) = 0$, is self-adjoint.

3. Let us consider somewhat further the "momentum operator", $p = \frac{1}{i}\frac{d}{dx}$, discussed briefly in the differential equation note. We let this operator be an operator on the Hilbert space of square-integrable (normalizable) functions, with $x \in [a, b]$.

   (a) Find the most general boundary condition such that p is Hermitian.

   (b) What is the domain, D_P, of p such that p is self-adjoint?

   (c) What is the situation when $[a, b] \to [-\infty, \infty]$? Is p bounded or unbounded?

4. Prove that the different systems of orthogonal polynomials are distinguished by the weight function and the interval. That is, the system of polynomials in $[a, b]$ is uniquely determined by $w(x)$ up to a constant for each polynomial.

5. We said that the recurrence relation for the orthogonal polynomials may be expressed in the form:

$$f_{n+1}(x) = (a_n + b_n x)\, f_n(x) - c_n f_{n-1}(x), \tag{255}$$

   see Eqn. 154. Try to verify.

6. We discussed some theorems for the qualitative behavior of classical orthogonal polynomials, and illustrated this with the one-electron atom radial wave functions. Now consider the simple harmonic oscillator (in one dimension) wave functions. The potential is

$$V(x) = \frac{1}{2}kx^2. \tag{256}$$

Thus, the Schrödinger equation is

$$-\frac{1}{2m}\frac{d^2}{dx^2}\psi(x) + \frac{1}{2}kx^2\psi(x) = E\psi(x). \tag{257}$$

Make a sketch showing the qualitative features you expect for the wave functions corresponding to the five lowest energy levels.

Try to do this with some care: There is really a lot that you can say in qualitative terms without ever solving the Schrödinger equation. Include a curve of the potential on your graph. Try to illustrate what happens at the classical turning points (that is, the points where $E = V(x)$).

7. Find the Green's function for the operator

$$L = \frac{d^2}{dx^2} + k^2, \tag{258}$$

where k is a constant, and with boundary conditions $u(0) = u(1) = 0$. For what values of k does your result break down? You may assume $x \in [0, 1]$.

8. An integral that is encountered in calculating radiative corrections in e^+e^- collisions is of the form:

$$I(t; a, b) = \int_a^b \frac{x^{t-1}}{1-x}dx, \tag{259}$$

where $0 \le a < b \le 1$, and $t \ge 0$.

Show that this integral may be expressed in terms of the hypergeometric function ${}_2F_1$. Make sure to check the $t = 0$ case.

9. We consider the Helmholtz equation in three dimensions:

$$\nabla^2 u + k^2 u = 0 \tag{260}$$

inside a sphere of radius a, subject to the boundary condition $u(r = a) = 0$. Such a situation may arise, for example, if we are interested in the electric field inside a conducting sphere. Our goal is to find $G(\mathbf{x}, \mathbf{y})$ such that

$$(\nabla_x^2 + k^2)G(\mathbf{x}, \mathbf{y}) = \delta(\mathbf{x} - \mathbf{y}), \tag{261}$$

with $G(r = a, \mathbf{y}) = 0$. We'll do this via one approach in this problem, and try another approach in the next problem.

Find $G(\mathbf{x},\mathbf{y})$ by obtaining solutions to the homogeneous equation

$$(\nabla^2 + k^2)G = 0, \tag{262}$$

on either side of $r = |\mathbf{y}|$; satisfying the boundary conditions at $r = a$, and the appropriate matching conditions at $r = |\mathbf{y}|$.

10. We return to the preceding problem. This is the problem of the Helmholtz equation:

$$\nabla^2 u + k^2 u = 0 \tag{263}$$

inside a sphere of radius a, subject to the boundary condition $u(r = a) = 0$. Such a situation may arise, for example, if we are interested in the electric field inside a conducting sphere. Our goal is to find $G(\mathbf{x},\mathbf{y})$ such that

$$(\nabla_x^2 + k^2)G(\mathbf{x},\mathbf{y}) = \delta(\mathbf{x}-\mathbf{y}), \tag{264}$$

with $G(r = a, \mathbf{y}) = 0$.

In problem 9, you found $G(\mathbf{x},\mathbf{y})$ by obtaining solutions to the homogeneous equation

$$(\nabla^2 + k^2)G = 0, \tag{265}$$

on either side of $r = |\mathbf{y}|$; satisfying the boundary conditions at $r = a$, and the appropriate matching conditions at $r = |\mathbf{y}|$.

Now we take a different approach: Find G by directly solving $(\nabla_x^2 + k^2)G(\mathbf{x},\mathbf{y}) = \delta(\mathbf{x}-\mathbf{y})$. You should ignore the boundary conditions at first and obtain a solution by integrating the equation over a small volume containing $\mathbf{y}$. Then satisfy the boundary conditions by adding a suitable function $g(\mathbf{x},\mathbf{y})$ that satisfies $(\nabla_x^2+k^2)g(\mathbf{x},\mathbf{y}) = 0$ everywhere.

11. Let's continue our discussion of the preceding two problems. This is the problem of the Helmholtz equation:

$$\nabla^2 u + k^2 u = 0 \tag{266}$$

inside a sphere of radius a, subject to the boundary condition $u(r = a) = 0$. Our goal is to find $G(\mathbf{x},\mathbf{y})$ such that

$$(\nabla_x^2 + k^2)G(\mathbf{x},\mathbf{y}) = \delta(\mathbf{x}-\mathbf{y}), \tag{267}$$

with $G(r = a, \mathbf{y}) = 0$.

In problem10, you found $G(\mathbf{x},\mathbf{y})$ by directly solving $(\nabla_x^2+k^2)G(\mathbf{x},\mathbf{y}) = \delta(\mathbf{x}-\mathbf{y})$, ignoring the boundary conditions at first. This is called the "fundamental solution" because it contains the desired singularity structure, and hence has to do with the "source". Now find the fundamental solution by another technique: Put the origin at $\mathbf{y}$ and solve the equation

$$(\nabla_x^2 + k^2)f(\mathbf{x}) = \delta(\mathbf{x}), \tag{268}$$

by using Fourier transforms. Do you get the same answer as last week?

12. Referring still to the Helmholz problem (problems 10 – 11), discuss the relative merits of the solutions found in problems 9 and 10. In particular, analyze, by making a suitable expansion, a case where the problem 10 solution is likely to be preferred, stating the necessary assumptions clearly.

13. We noted that the Green's function method is applicable beyond the Sturm-Liouville problem. For example, consider the differential operator:

$$L = \frac{d^4}{dx^4} + \frac{d^2}{dx^2}. \tag{269}$$

As usual, we wish to find the solution to $Lu = -\phi$. Let us consider the case of boundary conditions $u(0) = u'(0) = u''(0) = u'''(0) = 0$.

   (a) Find the Green's function for this operator.

   (b) Find the solution for $x \in [0, \infty]$ and $\phi(x) = e^{-x}$.

   You are encouraged to notice, at least in hindsight, that you could probably have solved this problem by elementary means.

14. Using the Green's function method, we derived in class the time development transformation for the free-particle Schrödinger equation in one dimension:

$$U(x, y; t) = \frac{1}{\sqrt{2}}\left(1 - i\frac{t}{|t|}\right)\sqrt{\frac{m}{2\pi|t|}} \exp\left[\frac{im(x-y)^2}{2t}\right]. \tag{270}$$

This should have the property that if you do a transformation by time t, followed by a transformation by time $-t$, you should get back to where you started. Check whether this is indeed the case or not.

15. Using the Christoffel-Darboux formula, find the projection operator onto the subspace spanned by the first three Chebyshev polynomials.

16. We discussed the radial solutions to the "one-electron" Schrödinger equation. Investigate orthogonality of the result – are our wave functions orthogonal or not?

17. In class we considered the problem with the Hamiltonian

$$H = -\frac{1}{2m}\frac{d^2}{dx^2}. \tag{271}$$

Let us modify the problem somewhat and consider the configuration space $x \in [a, b]$ ("infinite square well").

(a) Construct the Green's function, $G(x, y; z)$ for this problem.

(b) From your answer to part (a), determine the spectrum of H.

(c) Notice that, using

$$G(x, y; z) = \sum_{k=1}^{\infty} \frac{\phi_k(x)\phi_k^*(y)}{\omega_k - z}, \tag{272}$$

the normalized eigenstate, $\phi_k(x)$, can be obtained by evaluating the residue of G at the pole $z = \omega_k$. Do this calculation, and check that your result is properly normalized.

(d) Consider the limit $a \to -\infty$, $b \to \infty$. Show, in this limit that $G(x, y; z)$ tends to the Green's function we obtained in class for this Hamiltonian on $x \in (-\infty, \infty)$:

$$G(x, y; z) = i\sqrt{\frac{m}{2z}}e^{i\rho|x-y|}. \tag{273}$$

18. Let us investigate the Green's function for a slightly more complicated situation. Consider the potential:

$$V(x) = \begin{cases} V & |x| \leq \Delta \\ 0 & |x| > \Delta \end{cases} \tag{274}$$

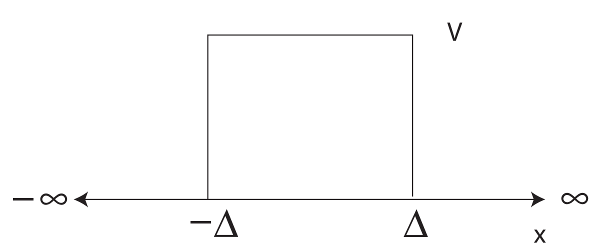

Figure 1: The "finite square potential".

(a) Determine the Green's function for a particle of mass m in this potential.

Remarks: You will need to construct your "left" and "right" solutions by considering the three different regions of the potential, matching the functions and their first derivatives at the boundaries. Note that the "right" solution may be very simply obtained from the "left" solution by the symmetry of the problem. In your solution, let

$$\rho = \sqrt{2m(z-V)} \tag{275}$$

$$\rho_0 = \sqrt{2mz}. \tag{276}$$

Make sure that you describe any cuts in the complex plane, and your selected branch. You may find it convenient to express your answer to some extent in terms of the force-free Green's function:

$$G_0(x,y;z) = \frac{im}{\rho} e^{i\rho_0|x-y|}. \tag{277}$$

(b) Assume $V > 0$. Show that your Green's function $G(x,y;z)$ is analytic in your cut plane, with a branch point at $z = 0$.

(c) Assume $V < 0$. Show that $G(x,y;z)$ is analytic in your cut plane, except for a finite number of simple poles at the bound states of the Hamiltonian.

19. In class, we obtained the free particle propagator for the Schrödinger equation in quantum mechanics:

$$U(x,t;x_0,t_0) = \frac{1}{\sqrt{2}}\left(1 - i\frac{t-t_0}{|t-t_0|}\right)\sqrt{\frac{m}{2\pi|t-t_0|}}\exp\left[\frac{im(x-x_0)^2}{2(t-t_0)}\right]. \tag{278}$$

Let's actually use this to evolve a wave function. Thus, let the wave function at time $t = t_0 = 0$ be:

$$\psi(x_0, t_0 = 0) = \left(\frac{1}{\pi a^2}\right)^{1/4} \exp\left(-\frac{x_0^2}{2a^2} + ip_0 x_0\right), \tag{279}$$

where a and p_0 are real constants. Since the absolute square of the wave function gives the probability, this wave function corresponds to a Gaussian probability distribution (i.e., the probability density function to find the particle at x_0) at $t = t_0$:

$$|\psi(x_0,t_0)|^2 = \left(\frac{1}{\pi a^2}\right)^{1/2} e^{-\frac{x_0^2}{a^2}}. \tag{280}$$

The standard deviation of this distribution is $\sigma = a/\sqrt{2}$. Find the probability density function, $|\psi(x,t)|^2$, to find the particle at x at some later (or earlier) time t. You are encouraged to think about the "physical" interpretation of your result.