Supplemental Notes on Mathematical Methods

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November 6, 2023

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CHAPTER 1

Sturm-Liouville Differential Equation

1.1 Motivation

Many of the problems we have studied follow from general properties of the Sturm-Lioville (SL) problem. In these problems, a system is governed by the differential equation of the form

$$\frac{\mathrm{d}}{\mathrm{d}x}\left[p(x)\frac{\mathrm{d}}{\mathrm{d}x}\right]\phi(x)+q(x)\phi(x)=-\lambda r(x)\phi(x) \tag{1.1}$$

for $x\in[a,b]$, where $a,b\in\mathbb{R}$ and some real functions p,q,r, where $p(x),r(x)>0$ for $x\in(a,b)$[1]. This is in essence an eigenvalue problem, where we would like to determine the eigenvalues λ and corresponding eigenfunctions $\phi(x)$ which satisfy Eq. (1.1) for a given set of p,q,r.

For example, the Schrödinger equation, Bessel's equation, and Legendre's equation all fall under this category. Clearly, the particular properties that determines a system's unique behavior depend on p,q,r, but the general methods by which we uncover these all follow the same generic trend which follow from general behaviors of systems with a Sturm-Lioville description.

1.2 Boundary Conditions

Since the Eq. (1.1) is a second-order differential equation, we have two linearly independent solutions $y_{1,2}$ for a given set of functions p,q,r, and a general solution $y=\alpha_1y_1+\alpha_2y_2$, where $\alpha_{1,2}$ are constants. These constants are determined by boundary conditions at $x=a,b$ by specifying (1) $y(a)$ and $y(b)$ [Dirichlet BCs], (2) $y'(a)$ and $y'(b)$ [Neumann BCs], or (3) $c_ay(a)+d_ay'(a)$ and $c_by(b)+d_by'(b)$ [Robin BCs]. For the most part, we focus on Dirichlet BCs

[1] Note that the endpoints are excluded here!

(e.g. specifying the value of the wave function) and Neumann (e.g. specifying the surface charge density). It is rare in the textbook problems that a linear combination of the function and its derivative are specified since these linear combinations are not usually related to a physical quantity. For the development of general properties, though, we will reference these kind of BCs, but Dirichlet and Neumann BCs are recovered by setting $d_{a,b} = 0$ and $c_{a,b} = 0$, respectively.

Finally, in some cases, a fourth distinct set of BCs can be specified, which are called periodic BCs. As the name suggests we either have $y(a) = y(b)$ or $y'(a) = y'(b)$.

1.3 Definitions

Let us define a couple of terms that will be used to identify the type of equation we consider.

1. A *regular* SL system is one such that homogeneous mixed BCs are given: $c_a y(a) + d_a y'(a) = 0$ and $c_b y(b) + d_b y'(b) = 0$
2. A *periodic* SL system is one such that periodic BCs are specified and $p(a) = p(b)$
3. A *singular* SL system is one where any of the following occur:
   - $p(a) = 0$, no BC at a is given, and the BC at b is homogeneous mixed (Note: solutions must be bounded at $x = a$)[2]
   - $p(b) = 0$, no BC at b is given, and the BC at a is homogeneous mixed (Note: solutions must be bounded at $x = a$)
   - $p(a) = p(b) = 0$ and no BCs are given (solutions must be bounded at both $x = a, b$.)
   - $a \to -\infty$ and $b \to \infty$ such that the equation is defined on $\mathbb{R}$ (Note: solutions must be square-integrable on $\mathbb{R}$)[3]

1.4 Properties of the Sturm-Liouville System

1.4.1 Sturm-Lioville Operator

Let $\mathcal{L}^2([a,b], r(x), \mathrm{d}x)$ be the Hilbert space of square integrable functions on the interval $[a, b]$ with inner product

$$(f, g) = \int_a^b r(x) f^*(x) g(x)\, \mathrm{d}x\,. \tag{1.2}$$

It is for this reason that $r(x)$ is sometimes denoted a *weight* function.

[2] A function f is bounded at x if $|f(x)| < M$ for some M.

[3] A function f is square-integrable if $\int_{-\infty}^{\infty} |f(x)|^2 < \infty$ (i.e. the integral is convergent and bounded).

Denote the linear differential operator

$$\hat{L} = -\frac{1}{r(x)}\left[\frac{\mathrm{d}}{\mathrm{d}x}p(x)\frac{\mathrm{d}}{\mathrm{d}x} + q(x)\right], \tag{1.3}$$

and let $\mathcal{H} \subset \mathcal{L}^2$ be the subspace of functions which are square integrable and satisfy a given set of BCs. The SL problem can then be stated as

$$\hat{L}\phi(x) = \lambda\phi(x), \tag{1.4}$$

and because of this relation we call L the SL operator. Effectively, we have explicitly rewritten Eq. (1.1) as an eigenvalue equation. We now study generally some properties of the SL operator and its spectrum and space of eigenfunctions.

1.4.2 Facts about solutions and eigenvalues of the Sturm-Lioville problem

Theorem 1: *The SL operator is self-adjoint.* Recall that the adjoint $A^\dagger$ of an operator A is defined by the equality $(A^\dagger f, g) = (f, Ag)$, and a self-adjoint operator is one such that $A^\dagger = A$. The proof is as follows for the SL operator. Consider the inner product

$$\begin{aligned}
(f, Lg) &= \int_a^b r f^* \hat{L} g \,\mathrm{d}x = \int_a^b f^* \left[-\frac{\mathrm{d}}{\mathrm{d}x}\Big(p\frac{\mathrm{d}}{\mathrm{d}x}\Big) + q \right] g \,\mathrm{d}x \\
&= -\int_a^b f^* \frac{\mathrm{d}}{\mathrm{d}x}\Big(p\frac{\mathrm{d}}{\mathrm{d}x}\Big) g \,\mathrm{d}x + \int_a^b [qf]^* g \,\mathrm{d}x \\
&= -\Big[f^* p g'\Big]_a^b + \int_a^b p\frac{\mathrm{d}f^*}{\mathrm{d}x}\frac{\mathrm{d}g}{\mathrm{d}x}\,\mathrm{d}x + \int_a^b [qf]^* g \,\mathrm{d}x \\
&= \left[p\left(\frac{\mathrm{d}f^*}{\mathrm{d}x}g - f^*\frac{\mathrm{d}g}{\mathrm{d}x}\right)\right]_a^b + \int_a^b \left\{\left[-\frac{\mathrm{d}}{\mathrm{d}x}p\frac{\mathrm{d}}{\mathrm{d}x} + q\right] f\right\}^* g \,\mathrm{d}x \\
&= \int_a^b (\hat{L}f)^* g \,\mathrm{d}x = (\hat{L}f, g).
\end{aligned} \tag{1.5}$$

We get rid of the boundary terms in order to have this proof work. It is a defining property of an SL system that the boundary term (which serves as the BC for the problem) vanishes. This is straightforward to see for homogeneous Dirichlet BCs ($f(a) = f(b) = g(a) = g(b) = 0$) and Neumann BCs ($f'(a) = f'(b) = g'(a) = g'(b) = 0$) and can be proven for each of the types of SL problems and BCs enumerated above.

Theorem 2: *The eigenvalues of $\hat{L}$ are real.* Suppose $\phi_\lambda \not\equiv 0$ is the function with corresponding eigenvalue λ. That is $\hat{L}\phi_\lambda = \lambda\phi_\lambda$. Since $\hat{L}$ is self-adjoint, we can write

$$\begin{aligned}
(\hat{L}\phi_\lambda, \phi_\lambda) &= (\phi_\lambda, \hat{L}\phi_\lambda) \\
(\lambda\phi_\lambda, \phi_\lambda) &= (\phi_\lambda, \lambda\phi_\lambda) \\
\lambda^*(\phi_\lambda, \phi_\lambda) &= \lambda(\phi_\lambda, \phi_\lambda) \\
\lambda^* &= \lambda
\end{aligned} \tag{1.6}$$

Theorem 3: *If ϕ_λ and ϕ_μ correspond to distinct eigenvalues λ and μ, then ϕ_λ and ϕ_μ are orthogonal (i.e. $(\phi_\lambda, \phi_\mu) = 0$).* The proof of this fact is straightforward. The eigenfunctions satisfy $\hat{L}\phi_\lambda = \lambda\phi_\lambda$ and $\hat{L}\phi_\mu = \mu\phi_\mu$. It follows then that

$$\begin{aligned}(\hat{L}\phi_\lambda, \phi_\mu) &= (\phi_\lambda, \hat{L}\phi_\mu)\\ \lambda(\phi_\lambda, \phi_\mu) &= \mu(\phi_\lambda, \phi_\mu).\end{aligned} \tag{1.7}$$

Rewriting we have

$$[\lambda - \mu](\phi_\lambda, \phi_\mu) = 0 \Rightarrow (\phi_\lambda, \phi_\mu) = 0 \tag{1.8}$$

since by assumption $\lambda \neq \mu$.

Theorem 4: *The spectrum of $\hat{L}$ is non-degenerate.* That is to say that if ϕ_1 and ϕ_2 correspond to the same eigenvalue, then $\phi_2 = c\phi_2$, or ϕ_1 and ϕ_2 are linearly dependent. We prove this by contradiction. Suppose that there exists $\phi_1 \neq \phi_2$ such that $\hat{L}\phi_{1,2} = \lambda\phi_{1,2}$. We then have

$$\begin{aligned}\phi_2\hat{L}\phi_1 - \phi_1\hat{L}\phi_2 &= -\frac{1}{r(x)}\left[\phi_2\frac{\mathrm{d}}{\mathrm{d}x}\Big(p\phi_1\Big) - \phi_1'\frac{\mathrm{d}}{\mathrm{d}x}\Big(p\phi_2'\Big)\right] = 0\\ &= -\frac{1}{r(x)}\frac{\mathrm{d}}{\mathrm{d}x}\underbrace{p(x)\Big[\phi_1'\phi_2 - \phi_1\phi_2'\Big]}_{W[\phi_1,\phi_2]} = 0.\end{aligned} \tag{1.9}$$

We then have

$$p(x)W[\phi_1(x), \phi_2(x)] = c. \tag{1.10}$$

Notice that for homogeneous BCs,

$$W[\phi_1(x), \phi_2(x)] = \frac{\mathrm{d}\phi_1}{\mathrm{d}x}\phi_2 - \phi_1\frac{\mathrm{d}\phi_2}{\mathrm{d}x} = 0. \tag{1.11}$$

This is simple to see for pure Dirichlet and Neumann BCs since either the function or the derivative is zero at the boundaries. Thus, we have a separable 1$^{\text{st}}$ order equation with solution

$$\phi_1(x) = c\phi_2(x). \tag{1.12}$$

Theorem 5: *The set of eigenfunctions is a basis for $\mathcal{H}$.* Equivalently, the set of eigenfunctions $\{\phi_\lambda\}$. Let us assume for now that $\hat{L}$ has a countable spectrum, allowing us to label the eigenfunctions by natural numbers such that eigenvalue λ_n corresponds to eigenfunction ϕ_n. A rigorous statement of completeness is this: if $\psi(x)$ is any function in $\mathcal{H}$,

$$\lim_{n\to N} ||\psi(x) - \sum_{k=1}^{n} c_k\phi_k||, \tag{1.13}$$

where N is the number of discrete eigenvalues in the spectrum of $\hat{L}$ (possibly infinite). Note that the coefficients $c_k = (\phi_k, \psi)$ and the norm $||\cdot||$ is defined as $||\psi|| = \sqrt{(\psi, \psi)}$. Another way of stating completeness is that

$$\sum_n \phi_n^*(x')\phi_n(x) = \delta(x - x'). \tag{1.14}$$

This is equivalent since any function $\psi \in \mathcal{H}$ can be expressed as

$$\psi(x) = \int_a^b \mathrm{d}x'\, \psi(x')\delta(x - x') = \sum_n \phi_n(x) \underbrace{\int_a^b \mathrm{d}x'\, \phi_n^*(x')\psi(x')}_{c_n}. \tag{1.15}$$

Note that there was no "proof" here. We really just posited that the eigenfunctions of $\hat{L}$ forms a complete basis. The proof is quite involved and requires a more formal and advanced treatment than is within the scope of this discussion. We will assume that the mathematicians who have proven this result are quite competent[4] and will simply take it as fact. It is essential that this theorem is true, though, since many of our problems hinge on the completeness of the eigenfunctions and our ability to expand a solution of an arbitrary SL problem in this basis.

1.5 Rodrigues' Formula

In this section, we are looking ahead a bit. In our studies of the Legendre polynomials, we were told that the l^{th} polynomial can be written as

$$P_l(x) = \frac{1}{2^l l!} \frac{\mathrm{d}^l}{\mathrm{d}x^l} \left(x^2 - 1\right)^l. \tag{1.16}$$

At the time, this formula seemed as if it were handed down from the heavens, requiring some divine inspiration that only applies to the case of Legendre polynomials. In some sense, this is true, but actually, for many physical systems, the eigenfunctions are some kind of polynomials, which in turn have their own "Rodrigues' formula".

Let us consider a simplified SL problem of the form

$$\frac{\mathrm{d}}{\mathrm{d}x}\left[p(x)\frac{\mathrm{d}\phi}{\mathrm{d}x}\right] = -\lambda r(x)\phi(x). \tag{1.17}$$

All we have done here is set $q(x) = 0$. Let us expand out the derivative in the first term as

$$p(x)\phi'' + p'(x)\phi' + \lambda r(x)\phi = 0. \tag{1.18}$$

Let us now present $p(x) = r(x)g(x)$. Our differential equation then becomes

$$r(x)g(x)\phi'' + [r'(x)g(x) + r(x)g'(x)]\phi' + \lambda r(x)\phi = 0. \tag{1.19}$$

Dividing by $r(x)$,

$$g(x)\phi'' + \left[\frac{r'(x)}{r(x)}g(x) + g'(x)\right]\phi' + \lambda\phi = 0. \tag{1.20}$$

[4]This argument is a bit flippant and depends on the assumption that the probability of a mistake being missed in the proof going to zero as the number of people who validated it goes to infinity (law of large numbers).

We have arrived at an alternate (but equivalent) form for the SL equation. If we have a differential equation of the form

$$g(x)\phi'' + h(x)\phi' + \lambda\phi = 0, \tag{1.21}$$

we can multiply by a weight function $r(x)$ such that

$$h(x) = \frac{r'(x)}{r(x)} g(x) + g'(x), \tag{1.22}$$

Solving for the form of r needed to put the Eq. (1.21) into SL form, we have

$$\begin{aligned}
\frac{r'(x)}{r(x)} = \frac{1}{r}\frac{\mathrm{d}r}{\mathrm{d}x} &= \frac{h}{g} - \frac{1}{g}\frac{\mathrm{d}g}{\mathrm{d}x} \\
\int \frac{1}{r}\frac{\mathrm{d}r}{\mathrm{d}x}\,\mathrm{d}x = \ln r(x) &= \int \frac{h(x)}{g(x)}\,\mathrm{d}x - \ln g(x) \\
r(x) &= \frac{1}{g(x)} \exp\left(\int \frac{h(x)}{g(x)}\,\mathrm{d}x\right). \qquad (1.23)
\end{aligned}$$

At this point, we can now formulate the Rodrigues formula given an SL problem posed as Eq. (1.21). Let us restrict our attention to situations with $g(x) = g_2x^2 + g_1x + g_0$ and $h(x) = h_1x + h_0$ and polynomial solutions to the differential equation of the form

$$\phi_n(x) = \sum_{k=0}^{n} \alpha_k x^k. \tag{1.24}$$

We will see that these specifications actually encompass many of the different systems we encounter and hence are general enough for our purposes here. If these restrictions are satisfied, then we claim that we can write

$$\phi_n(x) = \frac{1}{r(x)} \frac{\mathrm{d}^n}{\mathrm{d}x^n}[r(x)g^n(x)], \tag{1.25}$$

which is in fact Rodrigues' formula in full generality.

We now want to embark on a proof of this fact, which ultimately means that we must show that Eq. (1.25) satisfies Eq. (1.21). The first step of the proof is to determine the value λ_n:

$$(g_2x^2 + g_1x + g_0)\sum_{k=2}^{n} k(k-1)\alpha_k x^{k-2} + (h_1x + h_0)\sum_{k=1}^{n} k\alpha_k x^{k-1} + \lambda_n \sum_{k=0}^{n} \alpha_k x^k = 0. \tag{1.26}$$

Looking at the n^{th} order term, we have

$$g_2n(n-1)\alpha_n + h_1n\alpha_n + \lambda_n\alpha_n = 0 \text{ or } \lambda_n = -g_2n(n-1) - h_1n. \tag{1.27}$$

Next, observe that

$$g[rg^n]' = g[r'g^n + nrg^{n-1}g'] = rg^n\left[r' + nr\frac{g'}{g}\right] = rg^n[(n-1)g' + h]. \tag{1.28}$$

If we differentiate this equation $n+1$ times and divide by r we have

$$\frac{1}{r}\frac{\mathrm{d}^{n+1}}{\mathrm{d}x^{n+1}}g[rg^n]' = \frac{1}{r}\frac{\mathrm{d}^{n+1}}{\mathrm{d}x^{n+1}}rg^n[(n-1)g'+h]$$
$$\frac{1}{r}\sum_{k=0}^{n+1}\binom{n+1}{k}\frac{\mathrm{d}^k g}{\mathrm{d}x^k}\frac{\mathrm{d}^{n+2-k}[rg^n]}{\mathrm{d}x^{n+2-k}} = \frac{1}{r}\sum_{k=0}^{n+1}\binom{n+1}{k}\frac{\mathrm{d}^{n+1-k}[rg^n]}{\mathrm{d}x^{n+1-k}}\frac{\mathrm{d}^k}{\mathrm{d}x^k}[(n-1)g'+h]$$
$$\frac{g}{r}\frac{\mathrm{d}^{n+2}[rg^n]}{\mathrm{d}x^{n+2}} + \frac{(n+1)g'}{r}\frac{\mathrm{d}^{n+1}[rg^n]}{\mathrm{d}x^{n+1}} + \frac{n(n+1)g''}{2r}\frac{\mathrm{d}^n[rg^n]}{\mathrm{d}x^n} =$$
$$\frac{(n-1)g'+h}{r}\frac{\mathrm{d}^{n+1}[rg^n]}{\mathrm{d}x^{n+1}} + \frac{(n+1)[(n-1)g''+h']}{r}\frac{\mathrm{d}^n[rg^n]}{\mathrm{d}x^n}.$$

Note that $g^{(3)}=0$ and $h^{(2)}=0$ because they are quadratic and linear, respectively, which leaves us with only the few terms above upon the application of Leibniz's rule for differentiation of products:

$$\frac{\mathrm{d}^n}{\mathrm{d}x^n}f(x)g(x) = \sum_{k=0}^{n}\binom{n}{k}f^{(k)}(x)g^{(n-k)}(x) = \sum_{k=0}^{n}\frac{n!}{k!(n-k)!}f^{(k)}(x)g^{(n-k)}(x). \tag{1.29}$$

We now combine terms with common derivatives

$$\begin{aligned}\frac{g}{r}\frac{\mathrm{d}^{n+2}[rg^n]}{\mathrm{d}x^{n+2}} &= \frac{[(n-1)g'+h]-(n+1)g'}{r}\frac{\mathrm{d}^{n+1}[rg^n]}{\mathrm{d}x^{n+1}} \\ &+ \frac{2(n+1)[(n-1)g''+h']-n(n+1)g''}{2r}\frac{\mathrm{d}^n[rg^n]}{\mathrm{d}x^n} \\ &= \frac{-2g'+h}{r}\frac{\mathrm{d}^{n+1}[rg^n]}{\mathrm{d}x^{n+1}} + \frac{(n-2)(n+1)g''+2(n+1)h'}{2r}\frac{\mathrm{d}^n[rg^n]}{\mathrm{d}x^n}.\end{aligned} \tag{1.30}$$

Let us move everything over to the left and rewrite some factors in terms of ϕ_n:

$$\frac{g}{r}\frac{\mathrm{d}^2}{\mathrm{d}x^2}[r\phi_n] + \frac{2g'-h}{r}\frac{\mathrm{d}}{\mathrm{d}x}[r\phi_n] - \Big[\frac{n^2-n-2}{2}g''+(n+1)h'\Big]\phi_n = 0$$
$$\frac{g}{r}[r\phi_n''+2r'\phi_n'+r''\phi_n] + \frac{2g'-h}{r}[r'\phi_n+r\phi_n'] - \Big[\frac{n^2-n-2}{2}g''+(n+1)h'\Big]\phi_n = 0$$
$$g\phi_n'' + \Big[2g\frac{r'}{r}+(2g'-h)\Big]\phi_n' + \Big[g\frac{r''}{r}+(2g'-h)\frac{r'}{r} - \Big(\frac{n^2-n-2}{2}g''+(n+1)h'\Big)\Big]\phi_n = 0. \tag{1.31}$$

Recall that $r'/r = (h-g')/g$ and similarly

$$g\frac{r''}{r} = -\frac{r'}{r}(2g'-h) - (g''-h'). \tag{1.32}$$

Plugging these into the equation above:

$$g\phi_n'' + h\phi_n' + \Big[\frac{r'}{r}(h-2g') - (g''-h') + \frac{r'}{r}(2g'-h) - \Big(\frac{n^2-n-2}{2}g''+(n+1)h'\Big)\Big]\phi_n = 0$$
$$g\phi_n'' + h\phi_n' - \Big(\frac{n^2-n}{2}g''+nh'\Big)\phi_n = 0. \tag{1.33}$$

Almost there! Let us just recall that $\lambda_n = -[g''n(n-1)/2 + nh']$, meaning

$$g\phi_n'' + h\phi_n' + \lambda_n \phi_n = 0, \tag{1.34}$$

which is exactly the simplified SL form we assumed ϕ_n satisfied in the first place, proving Rodrigues' formula[5].

[5] Note that there are usually pre-factors in front of the derivative when considering specific cases. Scaling by a constant (i.e. $\phi_n \to c\phi_n$) does not change anything except for normalization.

CHAPTER 2

Gamma Function

The Gamma function appears in many places, including our treatment of specific cases of the Sturm-Lioville problem and its solution. Before moving on then, we will take a look at the Gamma function and work out some of its useful properties in a more elaborate way than in our courses, which primarily highlighted its definition and properties without indicating how they arise.

2.1 Definition

The Gamma function is really an analytic continuation of the factorial function to the complex plane. Let us define

$$\Gamma(z) = \int_0^\infty x^{z-1} e^{-x} \, \mathrm{d}x \, . \tag{2.1}$$

It is simple to derive its defining recursion property via integration by parts

$$\Gamma(z+1) = \int_0^\infty x^z e^{-x} \, \mathrm{d}x = -x^z e^{-x}\Big|_0^\infty + z \int_0^\infty x^{z-1} e^{-x} = z\Gamma(z). \tag{2.2}$$

If $z \in \mathbb{N}$[1], then

$$\Gamma(n+1) = n\Gamma(n) = \ldots = n(n-1)\ldots(3)(2)(1)\Gamma(1) = n!. \tag{2.3}$$

Note that

$$\Gamma(1) = \int_0^\infty e^{-x} \, \mathrm{d}x = -e^{-x}\Big|_0^\infty = 1. \tag{2.4}$$

One important observation is that the integral definition above only applies to $z \in \mathbb{C}$[2] such that $\mathrm{Re}\{z\} \geq 0$. If $\mathrm{Re}(z) < 0$, then the integrand is divergent as

[1] If you are not familiar with this notation $\mathbb{N} = \{1, 2, 3, \ldots\}$ is just the set of natural numbers.

[2] The set $\mathbb{C}$ is just the set of complex numbers.

$x \to 0$. We can however, use analytic continuation again to define the Gamma function for z with negative real parts using Eq. (2.3):

$$\Gamma(z) = \frac{1}{z}\Gamma(z+1). \tag{2.5}$$

Essentially, one applies this recursion relation N times until $z + N \geq 0$.

2.2 Important Identities

A common value that is needed is $\Gamma(1/2)$. Putting this into Eq. (2.1), we have

$$\Gamma(1/2) = \int_0^\infty x^{-1/2} e^{-x}\,\mathrm{d}x\,. \tag{2.6}$$

It may not be immedately clear how to integrate this. For $z = n + 1/2$, it is useful to relate the Gamma function to even moments of the Gaussian integral. If we use the substitution $x = y^2$,

$$\begin{aligned}\Gamma\Big(n+\frac{1}{2}\Big) &= \int_0^\infty x^{(2n-1)/2} e^{-x}\,\mathrm{d}x = \int_0^\infty y^{2n-1} e^{-y^2}(2y\,\mathrm{d}y) \\ &= 2\int_0^\infty y^{2n} e^{-y^2}\,\mathrm{d}y = \int_{-\infty}^\infty y^{2n} e^{-y^2}\,\mathrm{d}y\,. \end{aligned} \tag{2.7}$$

A common an useful trick is to introduce a parameter α in the Gaussian, differentiate with respect to this parameter n times, and take $\alpha \to 1$:

$$\begin{aligned}\int_{-\infty}^\infty y^{2n} e^{-\alpha y^2}\,\mathrm{d}y &= (-1)^n \frac{\mathrm{d}^n}{\mathrm{d}\alpha^n}\int_0^\infty e^{-\alpha y^2} = (-1)^n \frac{\mathrm{d}^n}{\mathrm{d}\alpha^n}\sqrt{\frac{\pi}{\alpha}} \\ &= (-1)^n\sqrt{\pi}\frac{\mathrm{d}^n}{\mathrm{d}\alpha^n}\alpha^{-1/2} \\ &= (-1)^n(-1/2)(-1/2-1)\ldots(-1/2-(n-1))\sqrt{\pi}\alpha^{-1/2+n} \\ &= \frac{1}{2}\cdot\frac{3}{2}\cdots\frac{2n-1}{2}\sqrt{\pi}\alpha^{-(2n+1)/2} = \frac{(2n-1)!!}{2^n}\sqrt{\pi}\alpha^{-(2n+1)/2}, \end{aligned} \tag{2.8}$$

where we have defined the "double-factorial" as

$$(2n)!! = (2n)(2n-2)\ldots(2) \tag{2.9}$$

$$(2n+1)!! = (2n+1)(2n-1)\ldots(1). \tag{2.10}$$

Essentially, instead of multiplying consecutive integers one by one, we just multiply integers that are separated by 2 units until we reach either 2 or 1. You can also see that we step n down one unit at a time, which steps $2n$ and $2n+1$ down 2 units.

Taking $\alpha \to 1$, we finally have

$$\Gamma\Big(n+\frac{1}{2}\Big) = \frac{(2n-1)!!\sqrt{\pi}}{2^n} = \frac{(2n)!\sqrt{\pi}}{2^{2n}n!}. \tag{2.11}$$

The last equality comes from noticing that we can write

$$\begin{aligned}
\frac{(2n)!}{n!} &= \frac{(2n)(2n-1)(2n-2)(2n-3)\dots(3)(2)(1)}{n!} \\
&= \frac{(2n)(2n-2)\dots(2)}{n!}(2n-1)!! \\
&= \frac{2^n(n)(n-1)\dots(2)(1)}{n!}(2n-1)!! = 2^n(2n-1)!!. \qquad (2.12)
\end{aligned}$$

It immediately follows then that

$$\Gamma(1/2) = \sqrt{\pi}. \qquad (2.13)$$

This could be gleaned directly from Eq. (2.7) also since $\Gamma(1/2)$ is just the Gaussian integral.

An alternate derivation of this fact is just to exploit the recursion property:

$$\begin{aligned}
\Gamma(n+1/2) &= (n-1/2)\Gamma(n-1/2) \\
&= \left(n-\frac{1}{2}\right)\left(n-\frac{3}{2}\right)\dots\left(\frac{3}{2}\right)\left(\frac{1}{2}\right)\Gamma(1/2). \qquad (2.14)
\end{aligned}$$

This is certainly the more straightforward approach, but the method used above highlights some other useful tools.

Another fact that was thrown at us is the following:

$$\Gamma(z)\Gamma(1-z) = \frac{\pi}{\sin \pi z}. \qquad (2.15)$$

If you would like, you can take it as a fact. The proof of this will require a relatively lengthy development, but we will eventually get to the end result. Let us define the beta function

$$B(p,q) = \int_0^1 x^{p-1}(1-x)^{q-1}\,\mathrm{d}x\,. \qquad (2.16)$$

We claim that $B(p,q) = \Gamma(p)\Gamma(q)/\Gamma(p+q)$. Let us now prove this claim. Recall that we can write

$$\Gamma(z) = 2\int_0^\infty x^{2z-1}e^{-x^2}\,\mathrm{d}x\,. \qquad (2.17)$$

This was shown writing $z = n + 1/2$, but in fact, the transformation did not depend on this assumption – it only lead to our ability to evaluate it in closed form after the substitution. Thus,

$$\Gamma(p)\Gamma(q) = 4\int_0^\infty\int_0^\infty x^{2p-1}y^{2q-1}e^{-(x^2+y^2)}\,\mathrm{d}x\,\mathrm{d}y\,. \qquad (2.18)$$

Let us change to polar coordinates via $x = r\cos\phi$ and $y = r\sin\phi$

$$\Gamma(p)\Gamma(q) = 4\int_0^{\pi/2}\cos^{2p-1}(\phi)\sin^{2q-1}(\phi)\,\mathrm{d}\phi\int_0^\infty r^{2p+2q-1}e^{-r^2}\,\mathrm{d}r\,. \qquad (2.19)$$

Note that ϕ only goes from 0 to $\pi/2$ since we only integrate over the first quadrant. Let us look at the angular integral and make the substitution $x = \sin^2\phi$. Thus, $\cos\phi = \sqrt{1-x}$ and $\mathrm{d}x = 2\sin\phi\cos\phi\,\mathrm{d}\phi$

$$\begin{aligned}\int_0^{\pi/2} \cos^{2p-1}(\phi)\sin^{2q-1}(\phi)\,\mathrm{d}\phi &= \int_0^1 (1-x)^{p-1/2}x^{q-1/2}\frac{\mathrm{d}x}{2x^{1/2}(1-x)^{1/2}} \\ &= \frac{1}{2}\int_0^1 x^{q-1}(1-x)^{p-1}\,\mathrm{d}x \\ &= \frac{1}{2}\int_0^1 y^{p-1}(1-y)^{q-1}\,\mathrm{d}y = \frac{1}{2}B(p,q), \qquad (2.20)\end{aligned}$$

where in the second-to-last step, we made the substitution $y = 1-x$. Essentially, this substitution showed the reciprocity of the beta function arguments: $B(p,q) = B(q,p)$. Next, it should be clear that the radial integral

$$\int_0^\infty r^{2p+2q-1}e^{-r^2}\,\mathrm{d}r = \frac{1}{2}\Gamma(p+q). \qquad (2.21)$$

Putting it all together, we have

$$\Gamma(p)\Gamma(q) = B(p,q)\Gamma(p+q). \qquad (2.22)$$

Before we finally prove Eq. (2.15), we have another representation of the beta function. Making the substitution $x = y/(1+y)$, we have $y = x/(1-x)$ and

$$\begin{aligned}B(p,q) &= \int_0^\infty \frac{y^{p-1}}{(1+y)^{p-1}}\frac{1}{(1+y)^{q-1}}\frac{\mathrm{d}y}{(1+y)^2} \\ &= \int_0^\infty \frac{y^{p-1}}{(1+y)^{p+q}}\,\mathrm{d}y\,. \qquad (2.23)\end{aligned}$$

Now, we are ready to prove Eq. (2.15). Let $p = z$ and $q = 1-z$. Then, using the most recent representation of the beta function

$$\Gamma(z)\Gamma(1-z) = B(z,1-z)\Gamma(1) = B(z,1-z) = \int_0^\infty \frac{x^{z-1}}{1+x}\,\mathrm{d}x\,. \qquad (2.24)$$

We have already evaluated this integral via contour integration. I will evaluate it here again for completeness. We integrate over the contour shown in Fig. 1 with the analytic continuation $x \to w$:

$$\begin{aligned}2\pi i(-1)^{z-1} = &\int_{C_{R\to\infty}} \frac{w^{z-1}}{1+w}\,\mathrm{d}w + \int_\infty^0 \frac{x^{1-z}e^{i2\pi(z-1)}}{1+x}\,\mathrm{d}x \\ &+ \int_{C_{\epsilon\to 0}} \frac{w^{z-1}}{1+w}\,\mathrm{d}w + \int_0^\infty \frac{x^{z-1}}{1+x}\,\mathrm{d}x\,. \qquad (2.25)\end{aligned}$$

The left hand-side is just the residue of the integrand at the pole $w = -1$. Rearranging, we have

$$B(z,1-z)[1-e^{i2\pi z}] = -2\pi i e^{i\pi z} - \int_{C_{R\to 0}} \frac{w^{z-1}}{1+w}\,\mathrm{d}w - \int_{C_{\epsilon\to 0}} \frac{w^{z-1}}{1+w}\,\mathrm{d}w\,. \qquad (2.26)$$

Along the path C_R, we can write $w = Re^{i\phi}$, giving

$$\int_{C_{R\to 0}} \frac{w^{z-1}}{1+w}\,\mathrm{d}w = i\int_0^{2\pi} \frac{R^z e^{iz\phi}}{1+Re^{i\phi}}\,\mathrm{d}\phi\,. \tag{2.27}$$

Taking $R \Rightarrow \infty$, this is zero, restricting $0 < z < 1$. Recycling most of the work and replacing R with ϵ, it is trivial to see that the integral along the path $C_{\epsilon\to 0}$ is zero. Thus,

$$\Gamma(z)\Gamma(1-z) = B(z, 1-z) = \frac{-2\pi i e^{i\pi z}}{1-e^{i2\pi z}} = \pi\frac{2i}{e^{i\pi z}-e^{-i\pi z}} = \frac{\pi}{\sin \pi z}. \tag{2.28}$$

At the moment, it seems that this result only holds for $0 < z < 1$. If we are outside this interval, we can always use the reciprocity relation and find an integer N such that $w = z + n$ is inside the interval $(0, 1)$. Suppose $z > 1$, then there exists $N > 0$ such that $w = z - N$ and

$$\begin{aligned}
\Gamma(z)\Gamma(1-z) &= \Gamma(w+N)\Gamma(1-[w+N]) \\
&= (w+[N-1])(w+[N-2])\ldots w\Gamma(w) \\
&\times \frac{1}{1-[w+N]}\frac{1}{2-[w+N]}\cdots\frac{1}{N-[w+N]}\Gamma(1-w) \\
&= (-1)^N\Gamma(w)\Gamma(1-w) = (-1)^N\frac{\pi}{\sin \pi w} \\
&= (-1)^N\frac{\pi}{\sin[\pi(z-N)]} = (-1)^N\frac{\pi}{\sin \pi z \cos \pi N} = \frac{\pi}{\sin \pi z}
\end{aligned} \tag{2.29}$$

since $\cos \pi N = (-1)^N$. A similar logic can be applied for $z < 0$, so indeed, Eq. (2.15) applies for any complex z.

CHAPTER 3

Legendre's Differential Equation and Legendre Polynomials

3.1 Legendre's Sturm-Liouville problem

3.2 Derivation of the differential equation

Legendre polynomials appear when we solve for example Laplace's equation in the spherical coordinate representation. In particular, Legendre polynomials arise when there is azimuthal symmetry, and the associated Legendre polynomials arise when we consider the full angular decomposition of solutions. Let us see this organically. Laplace's equation is generically given as

$$\nabla^2\phi(\vec{\boldsymbol{r}}) = 0. \tag{3.1}$$

In spherical coordinates, the Laplacian operator is

$$\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]\psi(r,\theta,\phi) = 0. \tag{3.2}$$

If we pose a separable ansatz for the solution $\psi(r,\theta,\phi) = R(r)P(\theta)T(\phi)$, then the equation reduces to

$$\underbrace{\frac{\sin^2\theta}{R(r)}\frac{\mathrm{d}}{\mathrm{d}r}\left(r^2\frac{\mathrm{d}R(r)}{\mathrm{d}r}\right) + \frac{\sin\theta}{P(\theta)}\frac{\mathrm{d}}{\mathrm{d}\theta}\left(\sin\theta\frac{\mathrm{d}P(\theta)}{\mathrm{d}\theta}\right)}_{F(r,\theta)} + \underbrace{\frac{1}{T(\phi)}\frac{\mathrm{d}^2T(\phi)}{\mathrm{d}\phi^2}}_{G(\phi)} = 0. \tag{3.3}$$

It is clear from this that both functions F and G are constants with respect to ϕ. Let us have

$$G(\phi) = -m^2 \Rightarrow \frac{\mathrm{d}^2T}{\mathrm{d}\phi^2} + m^2T = 0 \Rightarrow T(\phi) = e^{\pm im\phi}, \tag{3.4}$$

We know that the form of the solution in ϕ must be periodic such that $T(\phi + 2\pi) = T(\phi)$[1]. This constraint forces $m \in \mathbb{Z}$[2].

From this constraint, we can also write

$$F(r,\theta) = m^2, \tag{3.5}$$

which leads to

$$\underbrace{\frac{1}{R(r)}\frac{\mathrm{d}}{\mathrm{d}r}\left(r^2\frac{\mathrm{d}R(r)}{\mathrm{d}r}\right)}_{H(r)} + \underbrace{\frac{1}{\sin\theta P(\theta)}\frac{\mathrm{d}}{\mathrm{d}\theta}\left(\sin\theta\frac{\mathrm{d}P(\theta)}{\mathrm{d}\theta}\right) - \frac{m^2}{\sin^2\theta}}_{I(\theta)} = 0. \tag{3.6}$$

Again, H and I must be independent of r and θ, and we will set $I(\theta) = -\lambda$, which also means that $H(r) = \lambda$. Typically, we write the eigenvalue in a convenient form, but here we will remain oblivious to its form and recover the conventional $l(l+1)$ behavior later. For now, we ignore the radial dependence. The solution is not terribly difficult, but the associated Legendre polynomials we care about are the solutions to azimuthal angle dependent differential equation:

$$\frac{1}{\sin\theta}\frac{\mathrm{d}}{\mathrm{d}\theta}\left(\sin\theta\frac{\mathrm{d}P(\theta)}{\mathrm{d}\theta}\right) + \left[\lambda - \frac{m^2}{\sin^2\theta}\right]P(\theta) = 0. \tag{3.7}$$

This is equivalent to Legendre's equation, but we can write it in its canonical form via the substitution $x = \cos\theta$. The differential operator then transforms as

$$\frac{\mathrm{d}}{\mathrm{d}\theta} = \frac{\mathrm{d}x}{\mathrm{d}\theta}\frac{\mathrm{d}}{\mathrm{d}x} = \sin\theta\frac{\mathrm{d}}{\mathrm{d}x} = \sqrt{1-x^2}\frac{\mathrm{d}}{\mathrm{d}x}, \tag{3.8}$$

and therefore,

$$\left[\frac{\mathrm{d}}{\mathrm{d}x}(1-x^2)\frac{\mathrm{d}}{\mathrm{d}x} - \frac{m^2}{1-x^2}\right]P(x) = -\lambda P(x). \tag{3.9}$$

This equation is exactly of the SL form with $p(x) = 1 - x^2$, $q(x) = -m^2/(1-x^2)$, and $r(x) = 1$. It is clear since $p(\pm 1) = 0$ the boundary conditions are satisfied, and therefore, its solutions will be orthogonal in the sense that

$$(P_\lambda(x), P_\mu(x)) = \int_{-1}^{1} P_\lambda^*(x)P_\mu(x)\,\mathrm{d}x = 0 \tag{3.10}$$

if $\lambda \neq \mu$.

3.3 Series solution with $m = 0$

The differential equation Eq. (3.9) is generally true, but we can simplify our life a bit to begin by considering azimuthally symmetric solutions. That is, $m = 0$, giving

$$\frac{\mathrm{d}}{\mathrm{d}x}(1-x^2)\frac{\mathrm{d}P(x)}{\mathrm{d}x} + \lambda P_l(x) = 0. \tag{3.11}$$

[1]This is what led us to choose a negative constant for G in the first place too.
[2]The set $\mathbb{Z} = \{\ldots, -2, -1, 0, 1, 2\}$ is the collection of integers.

It will actually be seen later that we can obtain the solution for nonzero m from this special case.

It is not clear the above equation how to express P_l in terms of elementary functions, so we will solve the equation using Frobenius' method, which means that we write P_l as a power series

$$P(x) = \sum_{n=0}^{\infty} a_n x^{n+\gamma} \tag{3.12}$$

and solve for the coefficients a_n and γ such that P satisfies Legendre's equation. The introduction of γ allows the leading power of the expansion to potentially vary as well as make the powers non-integer. Putting this into Eq. (3.11), we have

$$\begin{gathered}
\frac{\mathrm{d}}{\mathrm{d}x}\left(1-x^2\right)\sum_{n=0}^{\infty}(n+\gamma)a_n x^{n+\gamma-1} + \sum_{n=0}^{\infty}\lambda a_n x^{n+\gamma} = 0 \\
\frac{\mathrm{d}}{\mathrm{d}x}\sum_{n=0}^{\infty}(n+\gamma)a_n x^{n+\gamma-1} - \frac{\mathrm{d}}{\mathrm{d}x}\sum_{n=0}^{\infty}(n+\gamma)a_n x^{n+\gamma+1} + \sum_{n=0}^{\infty}\lambda a_n x^{n+\gamma} \\
\sum_{n=0}^{\infty}(n+\gamma)(n+\gamma-1)a_n x^{n+\gamma-2} - \sum_{n=0}^{\infty}(n+\gamma)(n+\gamma+1)a_n x^{n+\gamma} + \sum_{n=0}^{\infty}\lambda a_n x^{n+\gamma} \\
\sum_{n=-2}^{\infty}(n+\gamma+2)(n+\gamma+1)a_{n+2}x^{n+\gamma} + \sum_{n=0}^{\infty}[\lambda-(n+\gamma)(n+\gamma+1)]a_n x^{n+\gamma}.
\end{gathered} \tag{3.13}$$

Shifting the indices of the first sum so that $n \to n+2$, we arrive at

$$\begin{aligned}
&\gamma(\gamma-1)a_0 x^{\gamma-2} + \gamma(\gamma+1)a_1 x^{\gamma-1} \\
&\quad + \sum_{n=0}^{\infty}\Big\{(n+\gamma+1)(n+\gamma+2)a_{n+2} + [\lambda-(n+\gamma)(n+\gamma+1)]a_n\Big\}x^{n+\gamma} = 0.
\end{aligned} \tag{3.14}$$

In order to have this expression be zero for every x, we must have the coefficients of each power of x be identically zero. For the first term, this means that

$$\gamma(\gamma-1) = 0 \Rightarrow \gamma = 0 \text{ or } 1. \tag{3.15}$$

These two solutions for γ are what give us our two solutions of the differential equation. For either value of γ, we must have

$$a_1 = 0. \tag{3.16}$$

since $(\gamma+1)(\gamma+2) > 0$. Focusing now on the coefficient inside the sum, we obtain the recurrence relation

$$a_{n+2} = \frac{(n+\gamma)(n+\gamma+1)-\lambda}{(n+\gamma+1)(n+\gamma+2)}a_n. \tag{3.17}$$

We can see immediately from this that the odd terms $a_{2n+1} = 0$ since these are recursively related to a_1.

This is where we determine the value of λ. The basis of the argument is that the power series solution must converge[3]. As a first pass, let us perform the

[3] Otherwise our power series is not really a function.

ratio test:

$$\lim_{n\to\infty}\left|\frac{a_{n+2}}{a_n}\right| = \lim_{n\to\infty}\frac{(n+\gamma)(n+\gamma+1)-\lambda}{(n+\gamma+1)(n+\gamma+2)} = 1. \tag{3.18}$$

The test is indeterminate, so we cannot conclude anything about the series about its convergence (or lack thereof). Another, more obscure test for us physicists, is the Gauss test. The theorem is this: *Consider a series $\sum_k a_k$ such that $a_k > 0$. Given a bounded function $B(k)$ as $k \to \infty$, if $|a_k/a_{k+1}| = 1 + A/n + B(n)/n^r$ with $r > 1$, then the series is divergent for $A \leq 1$ and convergent for $A > 1$.* We can expand the ratio of successive coefficients in the limit $n \to \infty$[4]

$$\frac{a_{2k}}{a_{2k+2}} = \frac{(2k+\gamma+1)(2k+\gamma+2)}{(2k+\gamma)(2k+\gamma+1)-\lambda} = 1 + \frac{1}{k} + \frac{\lambda-2\gamma}{4n^2} + \ldots. \tag{3.19}$$

We see from here that $A = 1$, implying that our series formally diverges for every λ if for every $n \geq 0$ there exists $N > n$ such that $a_N \neq 0$[5]. We, therefore, have to truncate our series such that there exists some $n = l$ with $a_l \neq 0$ but for each $n > l$ the coefficient $a_n = 0$. In terms of our recurrence relation, this says

$$a_{l+2} = \frac{(l+\gamma)(l+\gamma+1)-\lambda}{(l+\gamma+1)(l+\gamma+2)}a_l = 0 \Rightarrow \lambda = (l+\gamma)(l+\gamma+1). \tag{3.20}$$

For $\gamma = 0$, we clearly have $\lambda = l(l+1)$ for even $l > 0$ as expected, which makes

$$P(x;\gamma=0) = \sum_{n=0}^{l} a_n x^n = P_l(x), \tag{3.21}$$

which is a polynomial of degree l. For $\gamma = 1$, we have $\lambda = (l+1)(l+2)$ for even $l > 0$, but we can always redefine l such that $l \to l-1$, making l odd and $\lambda = l(l+1)$. Thus, our solutions for $\gamma = 1$

$$P(x;\gamma=1) = \sum_{n=0}^{l-1} a_n x^{n+1} = P_l(x). \tag{3.22}$$

We therefore have a full set of solutions for integers $l \geq 0$. As a final note, we fix the undetermined constant a_0 by enforcing $P_l(1) = 1$.

3.4 Rodrigues' Formula

In the chapter on Sturm-Liouville problems, we gave a general form for Rodrigues' formula. For the Legendre polynomials, we have $p(x) = 1-x^2$, $r(x) = 1$, and $g(x) = p(x)/r(x) = 1-x^2$. Thus, Rodrigues' formula for the Legendre polynomials is simply

$$P_l(x) = \mathcal{N}_l \frac{\mathrm{d}^l}{\mathrm{d}x^l}\left(1-x^2\right)^l. \tag{3.23}$$

[4] Tell wolfram the following: **expand (2k+gamma+1)(2k+gamma+2)/((2k+gamma)(2k+gamma+1) - lambda) as k -> infty**

[5] This is just a formal way of saying that the series includes an infinite number of nonzero coefficients.

All that remains now is to determine $\mathcal{N}_l$, which is done such that $P_l(1) = 1$. Before we do so, let us take $\mathcal{N}_l \to (-1)^l \mathcal{N}_l$ such that

$$P_l(x) = \mathcal{N}_l \frac{\mathrm{d}^l}{\mathrm{d}x^l} \left(x^2 - 1\right)^l. \tag{3.24}$$

This is convenient so that we can avoid doing the accounting for the extra factors of -1 each time we take a derivative, and we have the freedom to do this since any compensating factors will naturally arise in our later work.

Observe that by the binomial theorem (is it nicer to write x^{2k} or $x^{2(l-k)}$)

$$(x^2 - 1)^l = \sum_{k=0}^{l} \binom{l}{k} x^{2k}. \tag{3.25}$$

Taking the l^{th} derivative and evaluating at $x = 1$, we have

$$\begin{aligned} \frac{\mathrm{d}^l}{\mathrm{d}x^l} \left(x^2 - 1\right)^l \bigg|_{x=1} &= \sum_{k=\lfloor l/2 \rfloor}^{l} \frac{l!}{k!(l-k)!} (2k)(2k-1)\dots(2k-l+1) \\ &= \sum_{k=\lfloor l/2 \rfloor}^{l} \frac{l!(2k)!}{k!(l-k)!(2k-l)!} = \sum_{k=\lfloor l/2 \rfloor}^{l} \frac{l!}{(l-k)!(2k-l)!} 2^k (2k-1)!! \\ &. \end{aligned} \tag{3.26}$$

3.5 Generating Function

We have also found in Electricity & Magnetism that the function

$$g(x,t) = \frac{1}{\sqrt{1 - 2xt + t^2}} = \sum_{n=0}^{\infty} P_n(x) t^n. \tag{3.27}$$

That is, the coefficients of the power series expansion of g in powers of t are the Legendre polynomials we found in the previous section. We show that this is the case by proving that the coefficients of $g(x,t)$ satisfies Legendre's equation. First, we take

Appendices