Supplemental Notes on Mathematical Methods

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Contents

CHAPTER 1

Sturm-Liouville Differential Equation

1.1 Motivation

Many of the problems we have studied follow from general properties of the Sturm-Liouville (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-Liouville 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 $y = \alpha_1 y_1 + \alpha_2 y_2$, 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) $c_a y(a) + d_a y'(a)$ and $c_b y(b) + d_b y'(b)$ [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

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

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^{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 $\{\phi_\lambda\}$ is complete. 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 and will simply take it as fact[4]. 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 depends fundamentally on the law of large numbers, which is that the probability of a mistake being missed in the proof of this theorem goes to zero as the number of people who validated it goes to infinity. While it may not be satisfying, we at least can rest well knowing that many very smart people have taken a crack at proving this theorem and found it holds, so the chances of this fact being incorrect is effectively zero for our purposes.

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

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

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

$$g_2 n(n-1)\alpha_n + h_1 n\alpha_n + \lambda_n\alpha_n = 0 \text{ or } \lambda_n = -g_2n(n-1) - h_1 n. \tag{1.27}$$

Next, observe that

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

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

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

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:

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

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:

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

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].

1.6 Schlaefli integral and generating functions

We know from complex analysis that the n^{th} derivative of an analytic function is just

$$f^{(n)}(x) = \frac{n!}{2\pi i}\oint_C \frac{f(z)}{(z-x)^{n+1}}\,\mathrm{d}x\,, \tag{1.35}$$

where z is in the region bounded by C and f is analytic on and inside C. It quickly follows then that we can transform the generic Rodrigues formula such that

$$\phi_n(x) = \frac{1}{r(x)}\frac{n!}{2\pi i}\oint_C \frac{r(z)g^n(z)}{(z-x)^{n+1}}\,\mathrm{d}z\,. \tag{1.36}$$

In some cases, the integral representation of the SL solutions is useful in deriving a generating function $G(x,t)$ such that its power series expansion[6]

$$G(x,t) = \sum_n c_n\phi_n(x)t^n. \tag{1.37}$$

That is, the solutions to the SL problem (with some scalar) are just the coefficients of the expansion. If we put in the Schlaefli integral representation for $\phi_n(x)$, we have

$$G(x,t) = \sum_n c_n t^n \frac{n!}{2\pi i}\oint_C \frac{r(x)g^n(x)}{(z-x)^{n+1}}\,\mathrm{d}z\,. \tag{1.38}$$

This is not always useful since the integration must be possible to perform analytically, but there are a few cases of interest to us where we can use this to write down closed forms for the generating function. With such a function then, we will be able to write down recurrence relations that are useful in solving many different types of problems.

[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.

[6] $G(x,t)$ here should not be confused with a Green function of some sort. Typically generating functions are denoted by $g(x,t)$, but alas, we have already used g in a way that would make things confusing by reusing it.

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

2.2.1 Half-integer arguments

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 $\alpha \to 1$:

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

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

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

It immediately follows then that

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

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:

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

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

2.2.2 Euler reflection formula

Another fact that was thrown at us is the following:

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

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

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

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

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

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,

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

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

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

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 $\mathrm{d}x = 2\sin\phi\cos\phi\,\mathrm{d}\phi$

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

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

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

Putting it all together, we have

$$\Gamma(p)\Gamma(q) = B(p,q)\Gamma(p+q). \tag{2.22}$$

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

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

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

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

We integrate over the contour shown in Fig. (2.1) with the analytic continuation $x \to w$:

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

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

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

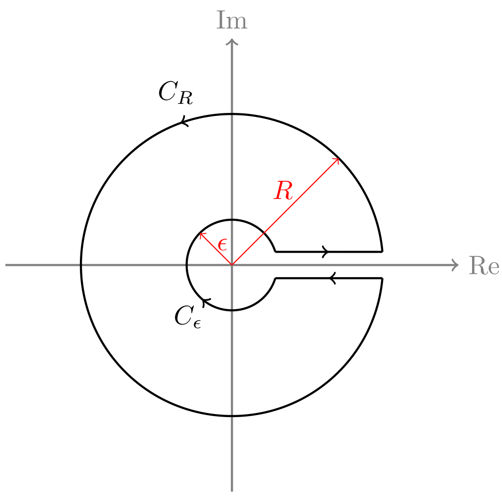

Figure 2.1: Contour definition for Eq. (2.25) to avoid multiple values along branch cut on the positive real axis.

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 $R \to \infty$, this is zero if we restrict $0 < z < 1$. 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.

2.2.3 Legendre duplication formula

In progress ...

CHAPTER 3

Legendre's Equation and Legendre Polynomials

3.1 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

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

In spherical coordinates, Laplace's equation 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].

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

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 since the associated Legendre polynomials we care about are the solutions to anglular portion of Laplace's 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,

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

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 $\lambda \neq \mu$.

3.2 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

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

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 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 convergence (or lack thereof) of the series. A more obscure test, yet equally valid one, is the Gauss test. The theorem is this: *Consider a series $\sum_k^\infty a_k$ such that $a_k > 0$. Given a bounded function $B(k)$ as $k \to \infty$, if $|a_k/a_{k+1}| = 1 + A/k + B(k)/k^r$ 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]

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

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 $P_l(1) = 1$.

3.3 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

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

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

[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 $P_l(1) = 1$. Observe that by the binomial theorem

$$(1-x^2)^l = \sum_{k=0}^{l} \binom{l}{k} (-x^2)^{l-k} = (-1)^l \sum_{k=0}^{l} \binom{l}{k} (-1)^k x^{2(l-k)}. \tag{3.24}$$

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

$$\begin{aligned}
\frac{\mathrm{d}^l}{\mathrm{d}x^l}\left(1-x^2\right)^l\Big|_{x=1} &= (-1)^l \sum_{k=0}^{\lfloor l/2 \rfloor} \binom{l}{k} (-1)^k (2l-2k)(2l-2k-1)\dots(2l-2k-l+1) \\
&= (-1)^l \sum_{k=0}^{\lfloor l/2 \rfloor} \frac{l!}{k!(l-k)!} \frac{[2(l-k)]!}{(l-2k)!} (-1)^k \\
&= (-1)^l l! \sum_{k=0}^{\lfloor l/2 \rfloor} \frac{(-1)^k}{k!(l-2k)!} \frac{2^{2(l-k)}}{\sqrt{\pi}} \Gamma([l-k]+1/2) \\
&= (-1)^l 2^l l! \sum_{k=0}^{\lfloor l/2 \rfloor} \frac{1}{\sqrt{\pi}} \frac{(-1)^k 2^{l-2k}}{k!(l-2k)!} \Gamma(l-k+1/2) \\
&= (-1)^l 2^l l! = \frac{1}{\mathcal{N}_l}.
\end{aligned} \tag{3.25}$$

At the moment, I do not have a derivation of the fact that the sum in the second-to-last-line gives 1. I plugged it into Wolfram, and it magically produced the result. We will take it at the moment unless some inspiration strikes that allows me to prove this without a computer algebra system. Anyway, putting this into Eq. (3.23), we find the result

$$P_l(x) = \frac{1}{2^l l!} \frac{\mathrm{d}^l}{\mathrm{d}x^l} \left(x^2-1\right)^l. \tag{3.26}$$

3.4 Generating Function

In a previous section, we have seen that we can write a generating function for the Legendre polynomials as

$$g(x,t) = \sum_{l=0}^{\infty} t^n \frac{l!}{2\pi i} \frac{1}{2^l l!} \oint_C \frac{(z^2-1)^l}{(z-x)^{l+1}} \, \mathrm{d}z \,. \tag{3.27}$$

We now pull the sum into the integral and use the geometric sum formula (forcing the contour small enough such that the sum is convergent[6]) such that

$$\begin{aligned}
g(x,t) &= \frac{1}{2\pi i} \oint_C \frac{1}{z-x} \sum_{l=0}^{\infty} \left(\frac{t(z^2-1)}{2(z-x)} \right)^l \\
&= \frac{1}{2\pi i} \oint_C \frac{2}{2(z-x) - t(z^2-1)} \\
&= \frac{1}{2\pi i} \left[-\frac{2}{t} \oint_C \left(z^2 - \frac{2}{t} z - \frac{2x-t}{t} \right)^{-1} \right].
\end{aligned} \tag{3.28}$$

[6]The condition is formally that $|t(z^2-1)/[2(z-x)]| < 1$

Notice that we can write

$$z^2 - \frac{2}{t}z - \frac{2x-t}{t} = (z-z_+)(z-z_-), \tag{3.29}$$

where

$$z_\pm = \frac{1}{t} \pm \sqrt{\frac{1}{t^2} - \frac{2x-t}{t}} = \frac{1}{t}\left[1 \pm \sqrt{1-2xt+t^2}\right]. \tag{3.30}$$

We now just have to apply the residue theorem to evaluate the integral. By forcing the contour to be small enough so that the sum converged, we made it so that only the pole $z = z_-$ is enclosed by the contour[7]. Using this fact, we have

$$g(x,t) = -\frac{2}{t}\frac{1}{z_- - z_+} = \frac{2}{t}\frac{t}{2\sqrt{1-2xt+t^2}} = \frac{1}{\sqrt{1-2xt+t^2}}. \tag{3.31}$$

Eq. (3.31) is exactly the generating function we have been given in class. By definition, we have

$$g(x,t) = \frac{1}{\sqrt{1-2xt+t^2}} = \sum_{n=0}^{\infty} P_n(x)t^n, \tag{3.32}$$

and now, we can derive a slew of recurrence relations between the Legendre polynomials and their derivatives that will come in handy. First, it is clear that

$$g(1,t) = \frac{1}{\sqrt{1-2t+t^2}} = \frac{1}{1-t} = \sum_{n=0}^{\infty} t^n, \tag{3.33}$$

which gives that $P_n(1) = 0$ as needed. Additionally, we can determine $P_n(-1)$ in the same way:

$$g(-1,t) = \frac{1}{1+t} = \sum_{n=0}^{\infty}(-1)^n t^n. \tag{3.34}$$

We can also determine $P_n(0)$

$$g(0,t) = \frac{1}{\sqrt{1+t^2}} = \sum_{n=0}^{\infty}(-1)^n \frac{(2n-1)!!}{(2n)!!}t^{2n}. \tag{3.35}$$

This says that $P_{2n+1}(0) = 0$ and $P_{2n}(0) = (-1)^n(2n-1)!!/(2n)!!$.

Next, we derive the three-term recurrence formula. First, we take the derivative of g with respect to t:

$$\frac{\partial g}{\partial t} = \frac{x-t}{(1-2xt+t^2)^{3/2}} = \frac{x-t}{1-2xt+t^2}g(x,t) = \sum_{n=0}^{\infty} nP_n(x)t^{n-1}. \tag{3.36}$$

[7] This is a subtle point: for the convergence condition above if x and $|t|$ are small, then $z_+ \approx 2/t \to \infty$ and $z_- \approx 0$. It is an important point though because otherwise the integration gives zero if neither pole or both poles are enclosed.

Thus,

$$
\begin{aligned}
(x-t)\sum_{n=0}^{\infty} P_n(x)t^n &= (1-2xt+t^2)\sum_{n=0}^{\infty} nP_n(x)t^{n-1}\\
\sum_{n=0}^{\infty} nP_n(x)t^{n-1} - \sum_{n=0}^{\infty}(2n+1)xP_n(x)t^n + \sum_{n=0}^{\infty}(n+1)P_n(x)t^{n+1} &= 0\\
\sum_{n=0}^{\infty}(n+1)P_{n+1}(x)t^n - \sum_{n=0}^{\infty}(2n+1)xP_n(x)t^n + \sum_{n=1}^{\infty} nP_{n-1}(x)t^n &\\
[P_1(x)-xP_0(x)] + \sum_{n=1}^{\infty}[(n+1)P_{n+1}(x)-(2n+1)xP_n(x)+nP_{n-1}(x)]t^n &= 0.
\end{aligned} \tag{3.37}
$$

We thus have a method to generate the Legendre polynomials iteratively. If we initiate the sequence with $P_0(x)=1$, then $P_1(x)=xP_0(x)=x$ and the higher order polynomials are given by

$$
P_{n+1}(x) = \frac{2n+1}{n+1}xP_n(x) - \frac{n}{n+1}P_{n-1}(x). \tag{3.38}
$$

If we instead take the derivative of g with respect to x, we obtain

$$
\frac{\partial g(x,t)}{\partial x} = \frac{t}{(1-2xt+t^2)^{3/2}} = \frac{t}{1-2xt+t^2}g(x,t) = \sum_{n=0}^{\infty} P_n'(x)t^n. \tag{3.39}
$$

Performing a series of manipulations

$$
\begin{aligned}
\sum_{n=0}^{\infty} P_n'(x)t^n - \sum_{n=0}^{\infty}[2xP_n'(x)+P_n(x)]t^{n+1} + \sum_{n=0}^{\infty} P_n'(x)t^{n+2} &= 0\\
P_0'(x) + [P_1'(x)-(2xP_0'(x)+P_0(x))]t + \sum_{n=0}^{\infty}[P_{n+2}'(x)-2xP_n'-P_n(x)-P_{n+1}(x)]t^{n+2} &= 0.
\end{aligned} \tag{3.40}
$$

Observing that $P_0'(x)=0$ and $P_1'(x)=1$, we have the following recurrence relation

$$
P_{n+1}'(x) + P_{n-1}'(x) = 2xP_n'(x) + P_n(x). \tag{3.41}
$$

We can rearrange Eq. (3.38), and take its derivative such that we find

$$
xP_n'(x) = \frac{n+1}{2n+1}P_{n+1}'(x) + \frac{n}{2n+1}P_{n-1}'(x) - P_n(x). \tag{3.42}
$$

Putting this into Eq. (3.41), we obtain

$$
\begin{aligned}
P_{n+1}'(x) + P_{n-1}'(x) &= \frac{2(n+1)}{2n+1}P_{n+1}'(x) + \frac{2n}{2n+1}P_{n-1}'(x) - P_n(x)\\
P_n(x) &= \frac{1}{2n+1}\Big[P_{n+1}'(x) - P_{n-1}'(x)\Big].
\end{aligned} \tag{3.43}
$$

This is another useful result. In particular, one thing we can derive with it is the following

$$\begin{aligned}\int_{-1}^{1} P_{n\neq 1}(x)\,\mathrm{d}x &= \frac{1}{2n+1}\left[P_{n+1}(x) - P_{n-1}(x)\right]_{-1}^{1} \\ &= \frac{1}{2n+1}\left[P_{n+1}(-1) - P_{n-1}(-1)\right] = \frac{(-1)^{n+1} - (-1)^{n-1}}{2n+1} = 0.\end{aligned} \tag{3.44}$$

If $n = 1$, then the integral is just 2. Similarly, if we adjust the lower bound to be zero

$$\int_{0}^{1} P_{n\neq 1}(x)\,\mathrm{d}x = \frac{P_{n+1}(0) - P_{n-1}(0)}{2n+1} = \begin{cases} 0 & \text{if } n = 2k \\ P_{2(k-1)}(0) - P_{2(k-1)}(0) & \text{if } n = 2k+1 \end{cases}. \tag{3.45}$$

If $n = 1$, the integral is just 1.

3.5 Normalization of Legendre polynomials

We already know from the chapter on SL theory that the Legendre polynomials are orthogonal in the sense that

$$(P_n, P_m) = \int_{-1}^{1} P_n(x) P_m(x)\,\mathrm{d}x = 0 \tag{3.46}$$

if $n \neq m$. In the case where $n = m$, though, we would like to determine

$$||P_n||^2 = (P_n, P_n) = \int_{-1}^{1} P_n^2(x)\,\mathrm{d}x\,. \tag{3.47}$$

We actually can do this by integrating the square of the generating function directly. That is

$$\begin{aligned}\int_{-1}^{1} g^2(x,t)\,\mathrm{d}x = \int_{-1}^{1} \frac{\mathrm{d}x}{1 - 2xt + t^2} &= \sum_{n,m=0}^{\infty} t^{n+m} \int_{-1}^{1} P_n(x) P_m(x)\,\mathrm{d}x \\ &= \sum_{n=0}^{\infty} t^{2n} \int_{-1}^{1} P_n^2(x)\,\mathrm{d}x\,.\end{aligned} \tag{3.48}$$

The integral on the left is simply solved by plugging it into Wolfram Alpha or pulling out an integral table

$$\int_{-1}^{1} \frac{\mathrm{d}x}{1 - 2xt + t^2} = \frac{1}{t}\ln\left(\frac{1+t}{1-t}\right). \tag{3.49}$$

We can now break out the Taylor expansion

$$\ln(1 \pm t) = \sum_{n=1}^{\infty} \frac{(-1)^n}{n} t^n, \tag{3.50}$$

to find

$$\frac{1}{t}\ln\left(\frac{1+t}{1-t}\right)=\sum_{n=1}^{\infty}\frac{(-1)^{n+1}-1}{n}t^{n-1}=\sum_{n=1}^{\infty}\frac{2}{2n-1}t^{2(n-1)}=\sum_{n=0}^{\infty}\frac{2}{2n+1}t^{2n}, \tag{3.51}$$

and equating this with the expansion of the generating function, we have

$$\sum_{n=0}^{\infty}\frac{2}{2n+1}t^{2n}=\sum_{n=0}^{\infty}t^{2n}(P_n,P_n). \tag{3.52}$$

Thus, in full generality,

$$(P_n,P_m)=\frac{2}{2n+1}\delta_{nm}. \tag{3.53}$$

3.6 Associated Legendre polynomials

The previous sections were quite a long discussion of Legendre polynomials, which are only a solution of the associated Legendre equation with $m=0$. Here we will see how to solve the equation

$$\frac{\mathrm{d}}{\mathrm{d}x}\left[(1-x^2)\frac{\mathrm{d}P(x)}{\mathrm{d}x}\right]+\left[\lambda-\frac{m^2}{1-x^2}\right]P(x)=0 \tag{3.54}$$

when m is nonzero. The first insight is to write $P(x)=(1-x^2)^r\mathcal{P}(x)$ such that the factor $1-x^2$ in the denominator of the last term is eliminated. Putting this into Eq. (3.9), we have

$$\begin{aligned}&\frac{\mathrm{d}}{\mathrm{d}x}\left[(1-x^2)^{r+1}\mathcal{P}'-2rx(1-x^2)^r\mathcal{P}\right]+\left[\lambda-\frac{m^2}{1-x^2}\right](1-x^2)^r\mathcal{P}=0\\&(1-x^2)^{r+1}\mathcal{P}''-2x[2r+1](1-x^2)^r\mathcal{P}'+\left[\lambda-\frac{1}{1-x^2}(m^2+2r[1-(2r+1)x^2])\right](1-x^2)^r\mathcal{P}=0.\end{aligned} \tag{3.55}$$

Dividing by $(1-x^2)^r$, we are left with

$$(1-x^2)\mathcal{P}''-2x(2r+1)\mathcal{P}+\left[\lambda-\frac{m^2+2r[1-(2r+1)x^2]}{1-x^2}\right]\mathcal{P}=0. \tag{3.56}$$

Observe that setting $r=m/2$ gets rid of this nuissance $1/(1-x^2)$ factor and leaves us with

$$(1-x^2)\mathcal{P}''-2x(m+1)\mathcal{P}'+[\lambda-m(m+1)]\mathcal{P}=0. \tag{3.57}$$

We can proceed as in the case of Legendre polynomials and solve via a series solution. This certainly would work, but it is incredibly tedious and not terribly englightening. Instead, we can stand on the shoulders of our predecessors and perform the following steps. Let us take Legendre's equation ($m=0$) and differentiate m times (note that this is implicitly assuming that m is positive):

$$\begin{aligned}&\frac{\mathrm{d}^m}{\mathrm{d}x^m}\left[(1-x^2)P_l''-2xP_l'+l(l+1)P_l\right]=0\\&(1-x^2)\frac{\mathrm{d}^{m+2}P_l}{\mathrm{d}x^{m+2}}-2mx\frac{\mathrm{d}^{m+1}P_l}{\mathrm{d}x^{m+1}}-m(m-1)\frac{\mathrm{d}^mP_l}{\mathrm{d}x^m}-2x\frac{\mathrm{d}^{m+1}P_l}{\mathrm{d}x^{m+1}}-2m\frac{\mathrm{d}^mP_l}{\mathrm{d}x^m}+l(l+1)\frac{\mathrm{d}^mP_l}{\mathrm{d}x^m}.\end{aligned} \tag{3.58}$$

If we set $\phi \equiv \mathrm{d}^{\mathrm{n}} P_l/\mathrm{d}x^n$, then ϕ satisfies

$$(1-x^2)\phi'' - 2x(m+1)\phi' + [l(l+1) - m(m+1)]\phi = 0, \tag{3.59}$$

which is exactly the same equation that $\mathcal{P}$ satisfied above with $\lambda = l(l+1)$. Thus, the solution to the associated Legendre equation is just

$$P_l^m(x) = (-1)^m (1-x^2)^{m/2} \frac{\mathrm{d}^m P_l(x)}{\mathrm{d}x^m}. \tag{3.60}$$

Note that the factor $(-1)^m$ is inserted by convention. Observe that we can include an additional constraint on the value of m now. Originally, we only restricted m to the integers, but now, it is clear that if $m > l$, then the m^{th} derivative of P_l, which is an l^{th} order polynomial, will be identically zero. We can obtain the solutions for $m < 0$ by inserting Rodrigues' formula for the Legendre polynomials, which gives

$$P_l^m = \frac{(-1)^m}{2^l l!}(1-x^2)^{m/2} \frac{\mathrm{d}^{l+m}}{\mathrm{d}x^{l+m}} \left(x^2-1\right)^l. \tag{3.61}$$

Let us now prove the relation between solutions for $m < 0$ and $m > 0$. For the negative m solutions, we have

$$\begin{aligned}
P_l^{-m} &= \frac{(-1)^m}{2^l l!}(1-x^2)^{-m/2} \frac{\mathrm{d}^{l-m}}{\mathrm{d}x^{l-m}} (x+1)^l (x-1)^l \\
&= \frac{(-1)^m}{2^l l!}(-1)^{-m/2}(x^2-1)^{-m/2} \sum_{k=0}^{l-m} \binom{l-m}{k} \frac{l!}{(l-k)!}(x+1)^{l-k} \frac{l!}{(m+k)!}(x-1)^{m+k} \\
&= \frac{(-1)^{m/2}}{2^l l!} \sum_{k=0}^{l-m} \frac{(l-m)!}{k!(l-m-k)!} \frac{l!}{(l-k)!} \frac{l!}{(m+k)!}(x+1)^{l-k-m/2}(x-1)^{k+m/2}.
\end{aligned} \tag{3.62}$$

Next, we do the same for the positive m solutions:

$$\begin{aligned}
P_l^m &= \frac{(-1)^m}{2^l l!}(1-x^2)^{m/2} \sum_{k=m}^{l} \binom{l+m}{k} \frac{l!}{(l-k)!} \frac{l!}{(k-m)!}(x+1)^{l-k}(x-1)^{k-m} \\
&= \frac{(-1)^{3m/2}}{2^l l!} \sum_{k=m}^{l} \frac{(l+m)!}{k!(l+m-k)!} \frac{l!}{(l-k)!} \frac{l!}{(k-m)!}(x+1)^{l-k+m/2}(x-1)^{k-m/2}.
\end{aligned} \tag{3.63}$$

If we shift indices such that $k \to k+m$, then

$$\begin{aligned}
P_l^m &= \frac{(-1)^{3m/2}}{2^l l!} \sum_{k=0}^{l-m} \frac{(l+m)!}{(k+m)!(l-k)!} \frac{l!}{(l-m-k)!} \frac{l!}{k!}(x+1)^{l-k-m/2}(x-1)^{k+m/2} \\
&= (-1)^m \frac{(l+m)!}{(l-m)!} P_l^{-m}.
\end{aligned} \tag{3.64}$$

This is equivalent to saying that

$$P_l^{-m}(x) = (-1)^m \frac{(l-m)!}{(l+m)!} P_l^m(x). \tag{3.65}$$

3.6.1 Normalization

When using the associated Legendre polynomials, which are related to spherical harmonics and hence are quite ubiquitous in physics applications, it is crucial to know their corresponding orthogonality relations (i.e. inner products)[8]:

$$(P_{l'}^m, P_l^m) = \frac{2}{2l+1}\frac{(l+m)!}{(l-m)!}\delta_{ll'}. \tag{3.66}$$

Very rarely though do we ever see the proof of this fact. The kronecker-delta factors are obvious given that solutions of an SL problem corresponding to distinct eigenvalues are orthogonal. It remains then to show that

$$(P_l^m, P_l^m) = \frac{2}{2l+1}\frac{(l+m)!}{(l-m)!}. \tag{3.67}$$

The first factor is exactly that of the Legendre polynomials ($m = 0$), and we have seen the second factor when relating the $-m$ and m associated Legendre polynomials to each other. This gives some indication for how to derive this fact then. First, we write explicitly the meaning of the inner product:

$$(P_l^m, P_l^m) = \int_{-1}^{1} [P_l^m(x)]^2 \,\mathrm{d}x\,. \tag{3.68}$$

We can relate one factor of P_l^m to its counterpart P_l^{-m} and write both in terms of the Rodrigues formula:

$$\begin{aligned}
(P_l^m, P_l^m) &= (-1)^m \frac{(l+m)!}{(l-m)!}\int_{-1}^{1} P_l^{-m}(x)P_l^m(x) \\
&= \frac{(-1)^m}{(2^l l!)^2}\frac{(l+m)!}{(l-m)!}\int_{-1}^{1}\left[(1-x^2)^{-m/2}\frac{\mathrm{d}^{l-m}}{\mathrm{d}x^{l-m}}\left(x^2-1\right)^l\right]\left[(1-x^2)^{m/2}\frac{\mathrm{d}^{l+m}}{\mathrm{d}x^{l+m}}\left(x^2-1\right)^l\right]\mathrm{d}x \\
&= \frac{(-1)^m}{(2^l l!)^2}\frac{(l+m)!}{(l-m)!}\int_{-1}^{1}\frac{\mathrm{d}^{l-m}}{\mathrm{d}x^{l-m}}\left(x^2-1\right)^l\frac{\mathrm{d}^{l+m}}{\mathrm{d}x^{l+m}}\left(x^2-1\right)^l\mathrm{d}x\,.
\end{aligned} \tag{3.69}$$

At this point, we will integrate by parts, taking derivatives successively from the second factor and appending them to the left factor until both are derivatives of order l. It will turn out that the boundary terms all vanish in the process:

$$\begin{aligned}
\int_{-1}^{1}\frac{\mathrm{d}^{l-m}}{\mathrm{d}x^{l-m}}(x^2-1)^l\frac{\mathrm{d}^{l+m}}{\mathrm{d}x^{l+m}}\left(x^2-1\right)^l\mathrm{d}x &= \frac{\mathrm{d}^{l-m}}{\mathrm{d}x^{l-m}}\left(x^2-1\right)^l\frac{\mathrm{d}^{l+m-1}}{\mathrm{d}x^{l+m-1}}\left(x^2-1\right)^l\Big|_{-1}^{1} \\
&\quad - \int_{-1}^{1}\frac{\mathrm{d}^{l-m+1}}{\mathrm{d}x^{l-m+1}}\left(x^2-1\right)^l\frac{\mathrm{d}^{l+m-1}}{\mathrm{d}x^{l+m-1}}\left(x^2-1\right)^l\mathrm{d}x \\
\ldots &= \sum_{k=1}^{m}(-1)^{k+1}\frac{\mathrm{d}^{l-m+(k-1)}}{\mathrm{d}x^{l-m+(k-1)}}\left(x^2-1\right)^l\frac{\mathrm{d}^{l+m-k}}{\mathrm{d}x^{l+m-k}}\left(x^2-1\right)^l\Big|_{-1}^{1} + (-1)^m\int_{-1}^{1}\left[\frac{\mathrm{d}^l}{\mathrm{d}x^l}\left(x^2-1\right)^l\right]^2\mathrm{d}x \\
&= (-1)^m(2^l l!)^2(P_l, P_l) = (-1)^m(2^l l!)^2\frac{2}{2l+1}.
\end{aligned} \tag{3.70}$$

[8]Note that $(P_l^{m'}, P_l^m) \neq 0$ generally since for fixed l the associated Legendre polynomials P_l^m and $P_l^{m'}$ both correspond to the same eigenvalue $l(l+1)$ of the SL equation.

Once we show why the boundary terms are zero, we will essentially be finished. The observation is simply that[9]

$$\frac{\mathrm{d}^{l-m+k}}{\mathrm{d}x^{l-m+k}}\left(x^2-1\right)^l = (x^2-1)^{m-k} f(x), \tag{3.71}$$

where $0 \leq k < m$ and $f(x)$ is some polynomial. Thus, since $m > k$, evaluating at $x = \pm 1$ always gives zero for the boundary terms.

Putting everything together, we finally have the normalization condition that was first quoted

$$(P_{l'}^m, P_l^m) = \frac{2}{2l+1}\frac{(l+m)!}{(l-m)!}\delta_{l'l}. \tag{3.72}$$

3.6.2 Parity

Let us define a parity transformation $f(\vec{\boldsymbol{r}}) \to f(-\vec{\boldsymbol{r}})$. Denote the operator which enacts this transformation as $\hat{\mathcal{P}}$. In many problems, parity is an important symmetry to consider, and many of these problems (e.g. quantum mechanics) involve spherical harmonics, which in turn depend on the associated Legendre polynomials. This will not be too complicated to derive. Consider the parity transformation of the associated Legendre polynomials, which we represent with the Rodrigues formula:

$$\hat{\mathcal{P}} P_l^m(x) = P_l^m(-x) = \frac{(-1)^m}{2^l l!}(1-x^2)^{m/2}\frac{\mathrm{d}^{l+m}}{\mathrm{d}(x)^{l+m}}\left(x^2-1\right)^l. \tag{3.73}$$

Clearly, the only place where the parity operation is non-trivial is on the derivative operator, but the image of the derivative under parity is not too difficult to derive:

$$\hat{\mathcal{P}}\frac{\mathrm{d}}{\mathrm{d}x} = \frac{\mathrm{d}}{\mathrm{d}(-x)} = \frac{\mathrm{d}(-x)}{\mathrm{d}x}\frac{\mathrm{d}}{\mathrm{d}x} = -\frac{\mathrm{d}}{\mathrm{d}x}. \tag{3.74}$$

Thus, taking $l+m$ derivatives equates to a factor $(-1)^{l+m}$ appended to the derivative operator under parity, yielding

$$P_l^m(-x) = (-1)^{l+m} P_l^m(x). \tag{3.75}$$

This is it for now. In the section on spherical harmonics, we will use this result to understand the action of the parity operator on the spherical harmonics.

[9]The observation is made rigorous via a proof by induction.

CHAPTER 4

Spherical Harmonics

This section will be fairly quick since in the previous chapter, we have already laid down most of the foundation. The spherical harmonics are functions $Y(\theta, \phi)$ which satisfy Laplace's equation, where θ and ϕ are the azimuthal and polar angles, respectively, in spherical coordinates:

$$r^2 \nabla^2 Y(\theta, \phi) = \frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \Big(\sin\theta \frac{\partial Y(\theta, \phi)}{\partial\theta} \Big) + \frac{1}{\sin^2\theta} \frac{\partial^2 Y(\theta, \phi)}{\partial\phi^2} = 0. \tag{4.1}$$

In the last chapter, we proceeded to solve this equation via a separable ansatz $Y(\theta, \phi) = P(\theta)T(\phi)$ and found that the azimuthal dependence is given by the associated Legendre polynomials $P(\theta) = P_l^m(\cos\theta)$ and the polar dependence is given by phase factors $e^{im\phi}$, where $l \geq 0$ and $-l \leq m \leq l$ are integers. The full separable solution is then just

$$Y_{lm}(\theta, \phi) = \mathcal{N}_{lm} P_l^m(\cos\theta) e^{im\phi}. \tag{4.2}$$

The normalization factor is fixed by requiring (as is conventional) that

$$\int \mathrm{d}\Omega \, Y^*_{l'm'}(\theta, \phi) Y^*_{lm}(\theta, \phi) = \delta_{l'l}\delta_{m'm}. \tag{4.3}$$

The orthogonality is already a given with the associated Legendre polynomials and phase factors. We can determine the normalization factor quite easily then:

$$\begin{aligned} 1 = \int_0^{2\pi} \mathrm{d}\phi \int_0^{\pi} \mathrm{d}\theta \sin\theta |Y_{lm}(\theta, \phi)|^2 &= \mathcal{N}_{lm}^2 (2\pi) \int_0^{\pi} \mathrm{d}\theta \sin\theta [P_l^m(\cos\theta)]^2 \\ &= \mathcal{N}_{lm}^2 (2\pi) \int_{-1}^{1} \mathrm{d}x \, [P_l^m(x)]^2 \\ &= \mathcal{N}_{lm} \frac{4\pi}{2l+1} \frac{(l+m)!}{(l-m)!}. \end{aligned} \tag{4.4}$$

Solving for $\mathcal{N}_{lm}$ then gives the normalized spherical harmonics as

$$Y_{lm}(\theta, \phi) = \sqrt{\frac{2l+1}{4\pi} \frac{(l-m)!}{(l+1)!}} P_l^m(\cos\theta) e^{im\phi}, \tag{4.5}$$

and that is the spherical harmonics in a nutshell.

4.1 Expansions in spherical harmonics

One final note is about the completeness of the spherical harmonics. Consistent with what we claimed in the Sturm-Liouville section, for any square-integrable function $f(\theta, \phi)$, we can expand it in spherical harmonics as

$$f(\theta, \phi) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} f_{lm} Y_{lm}(\theta, \phi), \tag{4.6}$$

where the coefficients are given through the orthonormality condition

$$f_{lm} = \int \mathrm{d}\Omega \, Y_{lm}^*(\theta, \phi) f(\theta, \phi). \tag{4.7}$$

If our function is rotationally symmetric about the z-axis then $f(\theta, \phi) = f(\theta)$ and only the $m = 0$ term survives, yielding an expansion in Legendre polynomials:

$$f(\theta) = \sum_{l=0}^{\infty} f_l P_l(\cos\theta) \tag{4.8}$$

with some constants absorbed into the coefficients

$$f_l = \frac{2l+1}{2} \int_0^{\pi} \mathrm{d}\theta \sin\theta P_l(\cos\theta) f(\theta). \tag{4.9}$$

4.2 Parity

In the section on associated Legendre polynomials, we introduced the parity operator, which is effectively a spatial inversion operator, and derived the action of this transformation on the associated Legendre functions. Here, we would like to do the same for the spherical harmonics. First, we must understand how the parity operator acts on the spherical coordinates themselves. Under parity, the cartesian coordinates transform trivially with a minus sign. We then easily obtain

$$r = \sqrt{x^2 + y^2 + z^2} \to r \tag{4.10}$$

$$. \tag{4.11}$$

The angles are perhaps a bit trickier since we must consider the domains of the trigonometric functions which define them. For example,

$$\phi = \arctan\left(\frac{y}{x}\right) \to \phi' = \arctan\left(\frac{-y}{-x}\right). \tag{4.12}$$

It is important not to simply cancel the minus signs without considering the fact that $\arctan x$ is only defined on $[-\pi/2, \pi/2]$, so it is only sensitive to the relative sign of x and y. On the other hand, though, the parity operator is a reflection through the origin, taking (x, y) into the point $(-x, -y)$, which is antiparallel to the original position vector projected into the xy-plane. Hence, this reflection through the origin is also equivalent to a 180° rotation about the z-axis, meaning the parity operator takes $\phi \to \phi + \pi$. Similarly, for the azimuthal angle

$$\theta = \arctan\left(\frac{\sqrt{x^2+y^2}}{z}\right) \to \theta' = \arctan\left(\frac{\sqrt{x^2+y^2}}{-z}\right). \tag{4.13}$$

We can see geometrically that the the parity operator is a reflection about the xy-plane with respect to z. Hence, if we define the angle ϑ as the angle that the position vector makes with the negative z-axis, then we have the simple relation $\vartheta + \theta = \pi$, and after the parity operation $\vartheta = \theta$, meaning that $\theta' = \pi - \vartheta = \pi - \theta$. As a summary, we then have

$$r \to r, \ \phi \to \phi + \pi, \ \text{and } \theta \to \pi - \theta. \tag{4.14}$$

Recall the spherical harmonics are given as

$$Y_{lm}(\theta, \phi) = \sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}} P_l^m(\cos\theta) e^{im\phi}, \tag{4.15}$$

so under parity

$$Y_{lm}(\theta, \phi) \to Y_{lm}(\pi - \theta, \phi + \pi) = \sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}} P_l^m(\cos(\pi - \theta)) e^{im(\phi+\pi)}. \tag{4.16}$$

Recall that $\cos(\pi - \theta) = -\cos\theta$ and $e^{im\pi} = \cos m\pi = (-1)^m$, so

$$\begin{aligned} Y_{lm}(\theta, \phi) \to Y_{lm}(\pi - \theta, \phi + \pi) &= (-1)^m \sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}} P_l^m(-\cos\theta) e^{im\phi} \\ &= (-1)^l Y_{lm}(\theta, \phi), \end{aligned} \tag{4.17}$$

where we have used $P_l^m(-x) = (-1)^{l+m} P_l^m(x)$.

CHAPTER 5

Bessel's equation and Bessel functions

We saw in the last few sections how the associated Legendre polynomials arose when solving Laplace's equation in spherical coordinates. In this section, we will see Bessel functions when solving Laplace's equation in cylindrical coordinates:

$$\frac{1}{s}\frac{\partial}{\partial s}\left(s\frac{\partial\psi}{\partial s}\right)+\frac{1}{s^2}\frac{\partial^2\psi}{\partial\phi^2}+\frac{\partial^2\psi}{\partial z^2}=0. \tag{5.1}$$

Again, we pose a separable ansatz $\psi(s,\phi,z)=R(s)T(\phi)Z(z)$, and plugging this in, we find

$$\frac{1}{sR}\frac{\mathrm{d}}{\mathrm{d}s}\left(s\frac{\mathrm{d}R}{\mathrm{d}s}\right)+\frac{1}{s^2T}\frac{\mathrm{d}^2T}{\mathrm{d}\phi^2}+\frac{1}{Z}\frac{\mathrm{d}^2Z}{\mathrm{d}z^2}=0. \tag{5.2}$$

It is clear from this that the two terms are independent of z, but the sign of this term is not immediately clear and depends on the boundary conditions of our particular problem. Let us write

$$\frac{1}{Z}\frac{\mathrm{d}^2Z}{\mathrm{d}z^2}=k^2 \tag{5.3}$$

with k not necessarily being real, meaning that k^2 can be any real number (positive, negative, or zero). Thus,

$$\frac{s}{R}\frac{\mathrm{d}}{\mathrm{d}s}\left(s\frac{\mathrm{d}R}{\mathrm{d}s}\right)+k^2s^2+\frac{1}{T}\frac{\mathrm{d}^2T}{\mathrm{d}\phi^2}=0. \tag{5.4}$$

The form of this term is exactly as in the spherical case since we must have $T(\phi+2\pi)=T(\phi)$, meaning that

$$\frac{1}{T}\frac{\mathrm{d}^2T}{\mathrm{d}\phi^2}=-\nu^2 \tag{5.5}$$

for $\nu\in\mathbb{Z}$. The equation for the s-dependence then becomes

$$s\frac{\mathrm{d}}{\mathrm{d}s}\left(s\frac{\mathrm{d}R}{\mathrm{d}s}\right)+(k^2s^2-\nu^2)R=0. \tag{5.6}$$

This equation is actually of the Sturm-Liouville type, but it will be easier to discuss after we form a solution. If we make the substitution $x = ks$, then the we have Bessel's equation

$$x\frac{\mathrm{d}}{\mathrm{d}x}\left(x\frac{\mathrm{d}R}{\mathrm{d}x}\right) + (x^2 - \nu^2)R = 0. \tag{5.7}$$

5.1 Bessel function of the first kind

As in the section on Legendre polynomials, we write R in a series as

$$R(x) = \sum_{n=0}^{\infty} a_n x^{n+\gamma}, \tag{5.8}$$

with $a_0 \neq 0$, which yields

$$\sum_{n=0}^{\infty}[(n+\gamma)^2 - \nu^2]a_n x^{n+\gamma} + \sum_{n=0}^{\infty} a_n x^{n+\gamma+2} = 0$$

$$(\gamma^2 - \nu^2)a_0 + [(\gamma+1)^2 - \nu^2]a_1 x + \sum_{n=0}^{\infty}\Big[[(n+2+\gamma)^2 - \nu^2]a_{n+2} + a_n\Big]x^{n+\gamma+2} = 0. \tag{5.9}$$

In order to have this expression be identically zero, we need

$$\gamma = \pm\nu \tag{5.10}$$

$$a_1 = 0 \tag{5.11}$$

$$\begin{aligned} a_{n+2} &= -\frac{1}{(n+2+\gamma)^2 - \gamma^2}a_n \\ &= -\frac{1}{(n+2)(n+2+2\gamma)}a_n. \end{aligned} \tag{5.12}$$

Note that by the recurrence relation all the odd terms are zero, so we can rewrite $n \to 2(n-1)$ such that

$$\begin{aligned} a_{2n} &= -\frac{1}{4n(n+\gamma)}a_{2(n-1)} \\ &= \Big(-\frac{1}{4}\Big)^n \frac{1}{[n(n-1)\dots(2)(1)][(n+\gamma)(n+\gamma-1)\dots(\gamma+1)]}a_0 \\ &= (-1)^n\Big(\frac{1}{2}\Big)^{2n}\frac{\gamma!}{n!(n+\gamma)!}a_0, \end{aligned} \tag{5.13}$$

and if we choose $a_0 = 1/[2^\gamma\Gamma(\gamma+1)]$ (this is only so that we can factor some terms and avoid carrying an overall factor), we obtain Bessel's function of the first kind:

$$J_\nu(x) = \Big(\frac{x}{2}\Big)^\nu \sum_{n=0}^{\infty}\frac{(-1)^n}{n!(n+\nu)!}\Big(\frac{x}{2}\Big)^{2n}, \tag{5.14}$$

where we allow ν to be any integer[1].

At this point, we cannot quite claim victory in the solution of Laplace's equation. If ν is in fact an integer, then J_ν and $J_{-\nu}$ are linearly dependent, meaning that these do not form a complete set of solutions to the Bessel equation. We can show this as follows. Let $\nu > 0$. Then,

$$\begin{aligned} J_{-\nu}(x) &= \sum_{n=\nu}^{\infty} \frac{(-1)^n}{n!(n-\nu)!} \left(\frac{x}{2}\right)^{2n-\nu} \\ &= \sum_{n=0}^{\infty} \frac{(-1)^{n+\nu}}{n!(n+\nu)!} \left(\frac{x}{2}\right)^{2n+\nu} \\ &= (-1)^\nu J_\nu(x). \end{aligned} \tag{5.15}$$

Note that the lowest index in the first equation is ν instead of zero since if $n < \nu$, then $(n-\nu)! = \Gamma(n-\nu+1) = 0$. Let us discuss some things related to the Bessel functions of the first kind and return in the next section to a discussion of a second solution for Bessel's equation.

5.1.1 Generating Function for integer ν

In the section on Legendre polynomials we derived exactly the generating function by writing down the Schlaefli integral with the Rodrigues formula definition of $P_n(x)$, summing the series, and then performing the contour integration. The situation for Bessel functions is not quite as nice. Our derivation of the general Rodrigues formula for a solution of a Sturm-Liouville equation requires that the solutions be polynomials, but we have already seen in the previous section that this is not the case for Bessel functions, which are infinite series. We actually neglected this point on convergence, but it should be simple to see that the series Eq. (5.14) is absolutely convergent for all x, ν:

$$\begin{aligned} &\lim_{n\to\infty} \left[\frac{1}{(n+1)!(n+1+\nu)!} \left(\frac{x}{2}\right)^{2(n+1)} \right] \left[n!(n+\nu)! \left(\frac{x}{2}\right)^{-2n} \right] \\ &\quad = \frac{x^2}{4} \lim_{n\to\infty} \frac{1}{n(n+\nu+1)} = 0. \end{aligned} \tag{5.16}$$

The generating function for Bessel functions of the first kind is given by the Laurent series

$$g(x,t) = e^{(x/2)(t-1/t)} = \sum_{n=-\infty}^{\infty} J_n(x) t^n. \tag{5.17}$$

While we will not derive this fact, we can show that the coefficients in the

[1] Actually, there are other systems with different BCs and behaviors which do not restrict ν to the integers, and since the series solution did not depend on ν other than in the indicial equation, this is true for any ν and $(n+\nu)! \to \Gamma(n+\nu+1)$

expansion of the generating function are in fact J_n. To do so, we will write

$$
\begin{aligned}
g(x,t) = e^{xt/2}e^{-x/2t} &= \left[\sum_{k=0}^{\infty}\frac{1}{k!}\left(\frac{xt}{2}\right)^k\right]\left[\sum_{l=0}^{\infty}\frac{1}{l!}\left(-\frac{x}{2t}\right)^l\right] \\
&= \sum_{k=0}^{\infty}\sum_{l=0}^{\infty}\frac{(-1)^l}{k!l!}\left(\frac{x}{2}\right)^{k+l}t^{k-l}. \qquad (5.18)
\end{aligned}
$$

We are almost there. Let us shift indices, defining $n = k - l$, giving

$$
g(x,t) = \sum_{n=-\infty}^{\infty}\left[\sum_{l=0}^{\infty}\frac{(-1)^l}{l!(l+n)!}\left(\frac{x}{2}\right)^{2l+n}\right]t^n = \sum_{n=-\infty}^{\infty}J_n(x)t^n, \qquad (5.19)
$$

which is exactly what we wanted to show.

5.1.2 Recurrence Relations

As we saw in the chapter on Legendre polynomials, the generating function is useful in deriving recurrence relations. We will not go through the exact derivations. The generic steps for deriving these relations are exactly like what we did for the Legendre polynomials. Differentiating with respect to t, we find

$$
J_{n-1}(x) + J_{n+1}(x) = \frac{2n}{x}J_n(x), \qquad (5.20)
$$

or alternatively, differentiating with respect to x, we find

$$
J_{n-1}(x) - J_{n+1}(x) = 2J_n'(x). \qquad (5.21)
$$

If we consider the previous equation with $n = 0$, we have

$$
J_{-1}(x) - J_1(x) = -2J_1(x) = 2J_0'(x) \Rightarrow J_0'(x) = -J_1(x). \qquad (5.22)
$$

We can also combine Eqs. (5.20)–(5.21) to derive more recurrence relations. First, let us add the two equations:

$$
\frac{2n}{x}J_n(x) + 2J_n'(x) = 2J_{n-1}(x). \qquad (5.23)
$$

Let us cancel the factor of 2 and multiply both sides by x^n, giving

$$
nx^{n-1}J_n(x) + x^nJ_n'(x) = \frac{\mathrm{d}}{\mathrm{d}x}[x^nJ_n(x)] = x^nJ_{n-1}(x). \qquad (5.24)
$$

If we instead subtract the equations and multiply by x^{-n}, we find instead that

$$
\frac{\mathrm{d}}{\mathrm{d}x}[x^{-n}J_n(x)] = -x^{-n}J_{n+1}(x). \qquad (5.25)
$$

Next, we can take the if we shift $n \to n+1$, we can write Eq. (5.23)

$$
J_n(x) = \frac{n+1}{x}J_{n+1}(x) + J_{n+1}'(x), \qquad (5.26)
$$

and doing a similar thing for the intermediate step of the derivation of Eq. (5.25), we find

$$
J_n(x) = \frac{n-1}{x}J_{n-1}(x) - J_{n-1}'(x). \qquad (5.27)
$$

5.1.3 General Solutions of Bessel's equation

Let us consider functions $Z_\nu(x)$ which satisfy the basic recurrence relations Eqs. (5.20)–(5.21). It is actually the case that this is sufficient to gurantee that Z_ν also satisfies Bessel's equation:

$$\begin{aligned}
&x^2 Z_\nu''(x) + x Z_\nu'(x) + (x^2-\nu^2) Z_\nu(x) \\
&\quad = \frac{x^2}{2}[Z_{\nu-1}'(x) - Z_{\nu+1}'(x)] + \frac{x}{2}[Z_{\nu-1}(x) - Z_{\nu+1}(x)] + (x^2-\nu^2)Z_\nu(x) \\
&\quad = \frac{x^2}{2}\Big[\Big(-Z_\nu(x) + \frac{\nu-1}{x}Z_{\nu-1}(x)\Big) - \Big(Z_\nu(x) - \frac{\nu+1}{x}Z_{\nu+1}(x)\Big)\Big] \\
&\quad + \frac{x}{2}[Z_{\nu-1}(x) - Z_{\nu+1}(x)] + (x^2-\nu^2)Z_\nu(x) \\
&\quad = -x^2 Z_\nu(x) + \frac{x}{2}\nu[Z_{\nu-1}(x) + Z_{\nu+1}(x)] + (x^2-\nu^2)Z_\nu(x) \\
&\quad = \frac{x}{2}\nu\frac{2\nu}{x}Z_\nu(x) - \nu^2 Z_\nu(x) = 0.
\end{aligned} \tag{5.28}$$

5.1.4 Integral representation of Bessel functions

Consider the following:

$$\begin{aligned}
\oint_C \mathrm{d}z\,\frac{e^{(x/2)(z-1/z)}}{z^{n+1}} &= \sum_m J_m(x)\oint_C \mathrm{d}z\,z^{m-n-1} = \sum_m J_m(x)[2\pi i\delta_{mn}] \\
&= J_n(x),
\end{aligned} \tag{5.29}$$

where we choose the contour C to encircle the singularity at $z=0$. If we choose the contour where $t = e^{i\theta}$, then we have

$$J_n(x) = \frac{1}{2\pi}\int_0^{2\pi} \mathrm{d}\theta\, e^{i(x\sin\theta - n\theta)}. \tag{5.30}$$

If x is real, then the imaginary part of the integral

$$\int_0^{2\pi} \sin(x\sin\theta - n\theta)\,\mathrm{d}\theta = 0 \tag{5.31}$$

and we have

$$J_n(x) = \frac{1}{2\pi}\int_0^{2\pi} \cos(x\sin\theta - n\theta)\,\mathrm{d}\theta\,. \tag{5.32}$$

5.1.5 Zeros of J_n

In many cases where Bessel functions are involved in the description of a physical system, the zeros of J_ν are intimately related to its important physical characteristics. While there is no closed form expression for the zeros, there are still a few important facts to be enumerated. The theorem of interest here is called the Sturm comparison theorem: *Let ϕ_1 and ϕ_2 be non-trivial solutions of equations*

$$\phi'' + q_1(x)\phi = 0 \tag{5.33}$$

$$\phi'' + q_2(x)\phi = 0, \tag{5.34}$$

respectively, on some interval $[a, b]$*, where* $q_{1,2}$ *are continuous functions such that* $q_1 \leq q_2$ *on* $[a, b]$*. Then between any two consecutive zeros* x_1 *and* x_2 *of* ϕ_1*, there exists at least one zero of* ϕ_2 *unless* $q_1(x) \equiv q_2(x)$ *on* (x_1, x_2)*.* We will not prove this theorem here since it is outside the scope of these notes. One note to make is that while the forms of Eq. (5.33)SL2-zeros does not appear to be of the standard SL form we are familiar with, it turns out that we can always make an appropriate substitution for ϕ to bring it into the standard SL form. For Bessel functions, let us demonstrate this fact by writing $J_\nu = x^{-1/2} y_\nu$. If we take derivatives of J_ν and write in terms of y_ν, we arrive at the differential equation which y_ν must satisfy:

$$y_\nu'' + \left[1 + \frac{1 - 4\nu^2}{4x^2}\right] y_\nu = 0. \tag{5.35}$$

Recall that $x > 0$ is the interval of interest for the Bessel equation. Let us consider a few cases then. First, if $0 < \nu < 1/2$, then $1 - 4\nu^2 > 0$ and $1 < 1 + (1 - 4\nu^2)/x^2$. Thus, we can compare to the differential equation $y'' + y = 0$, which has known solutions $\sin x$ and $\cos x$. We can write consecutive zeros of $\sin x$ for example as $((n-1)\pi, n\pi)$, where $n \in \mathbb{N}$, and we also can write consecutive zeros of $\cos x$ for example as $((n - 1/2)\pi, (n + 1/2)\pi)$. Thus, there must be at least one zero of y_ν, and therefore also J_ν, within these intervals, and furthermore, since there are an infinite number of these intervals, J_ν has an infinite number of zeros. Next, consider the case $\nu > 1/2$. We can consider $y'' + y = 0$ again. Let α and β be consecutive zeros of J_ν. It follows that there exists $n \in \mathbb{N}$ such that $\alpha < n\pi < \beta$, meaning that J_ν has an infinite set of non-trivial zeros.

5.1.6 Orthogonality

CHAPTER 6

Green Functions

In progress ...