Spherical Harmonics

by

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Laymen's Abstract

This report is about spherical harmonics, a mathematical tool used to understand patterns and shapes on the surface of a sphere, such as the Earth, or other shapes. You can think of them as the "building blocks" for describing how things vary across a spherical surface.

Just as musical notes can be combined to form complex sounds, spherical harmonics are used to combine simple mathematical patterns into more complicated ones. Scientists and engineers use them in many areas. For example, to represent 3D shapes, to model complex lighting in different environments, or to describe certain measurements on the atomics level.

In this report, we explore what spherical harmonics are, how they are built from simpler mathematical objects called polynomials, and why they are useful. Although the topic involves some advanced mathematics, the goal of this report is to offer a clear and structured introduction that helps readers gradually build their understanding.

Abstract

This report introduces spherical harmonics, functions defined on the surface of a sphere that play a central role in mathematical analysis, especially in problems with spherical symmetry. They appear in many fields, such as 3D representation within computer graphics, simulation light behaviour and angular momentum within quantum mechanics.

We begin by developing the theory from first principles. We look at what homogeneous harmonics polynomials are and explain how spherical harmonics arise by restricting these polynomials to the unit sphere. Using this we discuss properties such as orthogonality and dimension. We also discuss zonal harmonics, which are symmetric around a chosen axis.

In three dimensions, we solve Laplace's equation in spherical coordinates to derive explicit formulas for spherical harmonics. Associated Legendre polynomials will play a key role here. This directly connects with angular momentum, which will also be looked at in this report. This report aims to give students an introduction on spherical harmonics and how they can be used.

Contents

1
Introduction

Spherical harmonics arise naturally in problems with spherical symmetry in both theoretical and applied mathematics. They are special functions defined on the surface of a sphere. However, we will see that they can be extended to $\mathbb{R}^d$. This makes them especially useful for representing and analysing data defined on spherical domains. This report is intended as an accessible introduction to spherical harmonics, focusing on their mathematical foundation, while also looking at an application in quantum mechanics.

Spherical harmonics are used in modern applications that involve data or functions defined on the surface of a sphere. In 3D computer graphics and geometry, they help represent and process shapes and objects more efficiently, especially when working with curved surfaces. A recent study improved a method using spherical harmonics for 3D representation, leading to more accurate and stable results when analysing or reconstructing 3D shapes.[11]

They are also useful in simulating how light behaves in environments, particularly when dealing with complex lighting effects like reflections and polarization. Specialized versions of spherical harmonics make it possible to simulate these effects in a way that is both realistic and efficient, enabling techniques such as real-time rendering in visual applications.[3]

In quantum mechanics, spherical harmonics help describe the behaviour of certain particles, such as photons, especially when analysing their angular momentum. Spherical harmonics and angular momentum have a deep connection, as spherical harmonics help in removing uncertainty for particle measurements.[6] This application will be treated in this report.

In this report, we begin by introducing the abstract theory of spherical harmonics in chapter 2, starting with the definition of the unit sphere and homogeneous harmonic polynomials. We then explain how spherical harmonics are constructed from these polynomials and examine some of their key properties, such as orthogonality and dimension. Next, we look at a special type of spherical harmonics: zonal spherical harmonic. In chapter 3, we focus on the three-dimensional case, solving Laplace's equation in spherical coordinates to derive explicit formulas for spherical harmonics. In chapter 4 we discuss the application of spherical harmonics in angular momentum. Finally, we briefly reflect on possible extensions and applications of the theory in chapter 5. In the appendix, some useful results and definitions can be found that are used throughout the report.

2
Spherical Harmonics

This chapter introduces the space of spherical harmonics. We start by defining the domain of these functions, which is the unit sphere. Secondly, we introduce harmonic homogeneous polynomials. And lastly, we give the definition of spherical harmonics and give some examples of what these functions look like. This chapter is based on lecture notes written by Koornwinder[9] with some examples taken form an introductory book on spherical harmonics[1].

2.1. The unit sphere

Spherical harmonics are defined on the unit sphere in $\mathbb{R}^d$. We write this as follows,

$$S^{d-1} := \{\mathbf{x} \in \mathbb{R}^d \mid ||\mathbf{x}|| = 1\},$$

where $\mathbf{x}$ is a vector and $||\mathbf{x}|| = \sqrt{x_1^2 + \cdots + x_d^2}$ the euclidean norm. Here we thus write S^{d-1} for the unit sphere in $\mathbb{R}^d$. To rotate and reflect these vectors we introduce the set of all $d \times d$ orthogonal matrices,

$$O(d) := \{T \in M_d(\mathbb{R}) \mid T^T T = T T^T = I\},$$

where $M_d(\mathbb{R})$ is the set of all real $d \times d$ matrices. We use orthogonal matrices since these preserve the length of the vectors: $||T\mathbf{x}|| = ||\mathbf{x}||$ for $T \in O(d)$. To perform rotations or reflections we can define an action of $O(d)$ on S^{d-1}. However, for this we must first show that $O(d)$ is a group (recall the definitions of a group and an action in A.6 and A.7). For the group action we use the usual matrix multiplication. Then we have $I \in O(d)$ as the identity element. Furthermore, since $T^{-1} = T^T$ for all orthogonal matrices, we also have an inverse element. Lastly, for $A, B, C \in O(d)$ we have $A(BC) = (AB)C$, as this holds for all matrices. So indeed $O(d)$ forms a group.
Now we can define the action of $O(d)$ on S^{d-1}, which is a map $O(d) \times S^{d-1} \to S^{d-1}$ given by $(T, \mathbf{x}) \mapsto T\mathbf{x}$. The proof that this is indeed an action follows easily from matrix properties. Here, we have introduced vector rotation very rigorously, but note that it is indeed just matrix-vector multiplication.

2.2. Harmonic functions

We continue by defining the type of functions we will use to define the spherical harmonics. First, we restrict ourselves to the set of real-valued homogeneous polynomials. We define homogeneous polynomials in the following definition.

Definition 2.1. *A polynomial $f : \mathbb{R}^d \to \mathbb{R}$ is said to be homogeneous of degree n if it is a linear combination of the monomials*[1]

$$x_1^{n_1} x_2^{n_2} \cdots x_d^{n_d} \quad \text{such that } n_1 + n_2 + \cdots + n_d = n. \tag{2.1}$$

[1] A monomial is a polynomial with a single term.

The set of all homogeneous polynomials of degree n in $\mathbb{R}^d$ *is denoted as* $\mathcal{P}_n^d$.

Some concrete examples of homogeneous polynomials are shown in de following example.

Example 2.2.

1. $\mathcal{P}_2^2 = \{a_1x_1^2 + a_2x_2^2 + a_3x_1x_2 \mid a_i \in \mathbb{R}\}$,
2. $\mathcal{P}_2^3 = \{a_1x_1^2 + a_2x_2^2 + a_3x_3^2 + a_4x_1x_2 + a_5x_1x_3 + a_6x_2x_3 \mid a_i \in \mathbb{R}\}$,
3. $\mathcal{P}_3^2 = \{a_1x_1^3 + a_2x_2^3 + a_3x_1^2x_2 + a_4x_1x_2^2 \mid a_i \in \mathbb{R}\}$.

An important property of homogenous polynomials is that we have

$$f(r\mathbf{x}) = r^n f(\mathbf{x}) \quad \forall \mathbf{x} \in U,\ r \in \mathbb{R}.$$

We can see this by noting that every term of f is of the form (2.1), for which we see

$$(rx_1)^{n_1}(rx_2)^{n_2}\cdots(rx_d)^{n_d} = r^{n_1+\cdots+n_d}\left(x_1^{n_1}x_2^{n_2}\cdots x_d^{n_d}\right) = r^n\left(x_1^{n_1}x_2^{n_2}\cdots x_d^{n_d}\right).$$

Now for a vector $\mathbf{y} \in \mathbb{R}^d$ ($\mathbf{y} \neq \mathbf{0}$) we can write $\mathbf{y} = r\mathbf{x}$, where $r = ||\mathbf{y}||$ and $x = \frac{\mathbf{y}}{||\mathbf{y}||} \in S^{d-1}$ is the unit vector in the direction of $\mathbf{y}$. For any $f \in \mathcal{P}_n^d$ applying homogeneity gives the following,

$$f(\mathbf{y}) = f(r\mathbf{x}) = r^n f(\mathbf{x}). \tag{2.2}$$

Thus, once we know the values of a homogenous polynomial on the unit sphere, its values can be immediately determined on $\mathbb{R}^d$. To determine the dimension of $\mathcal{P}_n^d$, we need to count the number of monomials of degree n, as they form a basis for $\mathcal{P}_n^d$. This is equal to the number of ways to write $n = n_1 + \cdots + n_d$ with $n_1, ..., n_d \in \mathbb{Z}_{\geq 0}$. For this we can choose $d-1$ of the n_i, the last one is determined because the total must be n. We have a total power of n to divide over the variables so we get:

$$\dim\left(\mathcal{P}_n^d\right) = \binom{n+d-1}{d-1}. \tag{2.3}$$

This is not so straightforward to see, but to get a better understanding refer to the stars and bars problem. This is a well-known combinatorics problem, which is analogous to this problem. Another useful result for $f \in \mathcal{P}_n^d$ that will be used later, is the following lemma,

Lemma 2.3. *For* $f \in \mathcal{P}_n^d$ *we have*

$$\sum_{j=1}^{d} x_j \frac{\partial f(\mathbf{x})}{\partial x_j} = nf(\mathbf{x}). \tag{2.4}$$

Proof. Note that

$$nf(\mathbf{x}) = \frac{d}{dt}\left(t^n\right)\bigg|_{t=1} f(\mathbf{x}) = \frac{d}{dt} f(t\mathbf{x})\bigg|_{t=1} = \sum_{j=1}^{d} x_j \frac{\partial f(\mathbf{x})}{\partial x_j},$$

where we used homogeneity in the second step and the chain rule (stated in A.1) in the last step. □

We now introduce a natural action of $O(d)$ on $\mathcal{P}_n^d$, which describes how polynomials transform under rotations and reflections. It is defined by

$$\left(T \cdot f\right)(\mathbf{x}) := f\left(T^{-1}\mathbf{x}\right) \quad (f \in \mathcal{P}_n^d,\ T \in O(d)). \tag{2.5}$$

It is easily shown that this is indeed an action. Clearly we have $(I \cdot f)(\mathbf{x}) = f(I^{-1}\mathbf{x}) = f(\mathbf{x})$. Furthermore, for $A, B \in O(d)$, we see

$$((AB) \cdot f)(\mathbf{x}) = f((AB)^{-1}\mathbf{x}) = f(B^{-1}(A^{-1}\mathbf{x})) = (B \cdot f)(A^{-1}\mathbf{x}) = (A \cdot (B \cdot f))(\mathbf{x}).$$

Next, we give the definition of harmonic functions and show that for a harmonic function f, $T \cdot f$ is again harmonic.

Definition 2.4. *A function $f : U \to \mathbb{R}$, where $U \subseteq \mathbb{R}^d$ is open, is harmonic if it is twice continuously differentiable and*

$$\frac{\partial^2 f}{\partial x_1^2} + \frac{\partial^2 f}{\partial x_2^2} + \cdots + \frac{\partial^2 f}{\partial x_d^2} = 0. \tag{2.6}$$

This is usually written as: $\nabla^2 f = 0$ or $\Delta f = 0$, where Δ is called the Laplace operator. Furthermore, equation (2.6) *is called the Laplace equation. The set of all twice continuously differentiable functions on U is denoted as $C^2(U)$.*

Proposition 2.5. *If $T \in O(d)$ and $f \in C^2(\mathbb{R}^d)$ is harmonic, then $T \cdot f$ is again harmonic.*

Proof. We show that $\Delta(T \cdot f) = \Delta f = 0$. For this let $y = T^{-1}x \ (T \in O(d))$, then we need to show

$$\sum_{i=1}^{d} \left(\frac{\partial}{\partial x_i}\right)^2 = \sum_{j=1}^{d} \left(\frac{\partial}{\partial y_j}\right)^2$$

Indeed,

$$\frac{\partial}{\partial x_i} = \sum_{j=1}^{d} \frac{\partial y_j}{\partial x_i} \frac{\partial}{\partial y_j} = \sum_{j=1}^{d} \left(T^{-1}\right)_{j,i} \frac{\partial}{\partial y_j} = \sum_{j=1}^{d} T_{i,j} \frac{\partial}{\partial y_j},$$

where in the first equality we applied the chain rule. We obtain the second equality by observing that $y_j = \sum_{k=1}^{d} T^{-1}_{j,k} x_k$, so $\frac{\partial y_j}{\partial x_i} = (T^{-1})_{j,i}$. The last equality uses orthogonality: $T^{-1} = T^T$, so $(T^{-1})_{j,i} = T_{i,j}$. Now this implies that

$$\begin{aligned}
\sum_{i=1}^{d} \left(\frac{\partial}{\partial x_i}\right)^2 &= \sum_{i=1}^{d} \left(\sum_{j=1}^{d} T_{i,j} \frac{\partial}{\partial y_j}\right)^2 \\
&= \sum_{i=1}^{d} \sum_{j=1}^{d} \sum_{k=1}^{d} T_{i,j} T_{i,k} \frac{\partial}{\partial y_j} \frac{\partial}{\partial y_k} \\
&= \sum_{j=1}^{d} \sum_{k=1}^{d} \left(\sum_{i=1}^{d} T_{i,j} T_{i,k}\right) \frac{\partial}{\partial y_j} \frac{\partial}{\partial y_k}
\end{aligned}$$

Now note that $\sum_{i=1}^{d} T_{i,j} T_{i,k}$ is the dot product of column j and k and since T has orthonormal columns, we have that $\sum_{i=1}^{d} T_{i,j} T_{i,k}$ is equal to 1 if $i = j$ and equal to 0 if $i \neq j$. The triple sum thus reduces to $\sum_{j=1}^{d} \frac{\partial}{\partial y_j} \frac{\partial}{\partial y_j}$, from which we obtain

$$\sum_{i=1}^{d} \left(\frac{\partial}{\partial x_i}\right)^2 = \sum_{j=1}^{d} \left(\frac{\partial}{\partial y_j}\right)^2. \qquad \square$$

Having defined homogeneous polynomials and harmonic functions, we can define the space of real harmonic homogeneous polynomials on $\mathbb{R}^d$ of degree n:

$$\mathcal{H}_n^d := \{f \in \mathcal{P}_n^d \mid \Delta f = 0\}.$$

We follow with a lemma which shows that all functions in $\mathcal{H}_n^d$ containing a factor $||\mathbf{x}||^2$ are equal to zero. Next, the lemma will be used in a proposition relating $\mathcal{P}_n^d$ and $\mathcal{H}_n^d$.

Lemma 2.6. *Let $n \geq 2$, $f \in \mathcal{P}_{n-2}^d$ and $F(\mathbf{x}) := ||\mathbf{x}||^2 f(\mathbf{x})$. Then $F \in \mathcal{P}_n^d$ and if additionally $F \in \mathcal{H}_n^d$ we have $F = 0$*

Proof. Since for $f \in \mathcal{P}^d_{n-2}$ every element is of degree $n-2$, so clearly multiplying by $x_1^2+\cdots+x_d^2$ yields a function in $\mathcal{P}^d_n$. Now suppose $F \in \mathcal{H}^d_n$. To show $F = 0$, assume $F \neq 0$. Then there exists a maximal k $(1 \leq k \leq \frac{1}{2}n)$ such that $F(\mathbf{x}) = ||\mathbf{x}||^{2k} g(\mathbf{x})$ for some $g \in \mathcal{P}^d_{n-2k}$. In other words, we factor out $||\mathbf{x}||^2$ as many times as possible. We will compute $\Delta(||\mathbf{x}||^{2k} g(\mathbf{x}))$ to reach a contradiction. For this, first note that for general functions $p(\mathbf{x})$ and $q(\mathbf{x})$, by applying the product rule twice, we have

$$\frac{\partial^2}{\partial x_i^2}(fg) = f\frac{\partial^2 g}{\partial x_i^2} + 2\frac{\partial f}{\partial x_i}\frac{\partial g}{\partial x_i} + g\frac{\partial^2 f}{\partial x_i^2}.$$

Now summing over all i we get the Laplacian for a product of two functions,

$$\Delta(fg) = \sum_{i=1}^{d}\left(f\frac{\partial^2 g}{\partial x_i^2} + 2\frac{\partial f}{\partial x_i}\frac{\partial g}{\partial x_i} + g\frac{\partial^2 f}{\partial x_i^2}\right) = f\Delta g + 2\sum_{i=1}^{d}\frac{\partial f}{\partial x_i}\frac{\partial g}{\partial x_i} + g\Delta f.$$

Write $r := ||\mathbf{x}||$, then we can apply the above to the product $r^2 g(\mathbf{x})$ and see

$$0 = \Delta\left(r^{2k}\right)g(\mathbf{x}) + 2\sum_{i=1}^{d}\frac{\partial}{\partial x_i}\left(r^{2k}\right)\frac{\partial}{\partial x_i}g(\mathbf{x}) + r^{2k}\Delta g(\mathbf{x}). \tag{2.7}$$

Next we use that Δ acting on a function only depending on r acts as $\frac{d^2}{dr^2} + \frac{d-1}{r}\frac{d}{dr}$. We can show this by directly computing. For a general function $p(r)$, we have

$$\frac{\partial}{\partial x_i}p(r) = \frac{dp(r)}{dr}\frac{\partial r}{\partial x_i} = \frac{dp(r)}{dr}\frac{2x_i}{2r} = \frac{dp(r)}{dr}\frac{x_i}{r}.$$

This yields

$$\frac{\partial^2}{\partial x_i^2}p(r) = \frac{d}{dx_i}\left(\frac{dp(r)}{dr}\;\frac{x_i}{r}\right) = \frac{d^2p(r)}{dr^2}\cdot\left(\frac{x_i}{r}\right)^2 + \frac{dp(r)}{dr}\cdot\frac{d}{dx_i}\left(\frac{x_i}{r}\right),$$

where

$$\frac{d}{dx_i}\left(\frac{x_i}{r}\right) = \frac{r - x_i\frac{x_i}{r}}{r^2} = \frac{r^2 - x_i^2}{r^3}.$$

Now we sum over all i and see,

$$\Delta p(r) = \sum_{i=1}^{d}\frac{\partial^2}{\partial x_i^2}p(r) = \frac{d^2p(r)}{dr^2}\sum_{i=1}^{d}\frac{x_i^2}{r^2} + \frac{dp(r)}{dr}\sum_{i=1}^{d}\frac{r^2 - x_i^2}{r^3}.$$

Finally, we compute the two sums:

$$\sum_{i=1}^{d} x_i^2 = r^2 \Rightarrow \sum_{i=1}^{d}\frac{x_i^2}{r^2} = 1$$
$$\sum_{i=1}^{d}(r^2 - x_i^2) = \sum_{i=1}^{d} r^2 - \sum_{i=1}^{d} x_i^2 = dr^2 - r^2 = (d-1)r^2 \Rightarrow \sum_{i=1}^{d}\frac{r^2 - x_i^2}{r^3} = \frac{d-1}{r}.$$

We apply this to $\Delta\left(r^{2k}\right)$ in (2.7). Furthermore, we can compute $\frac{\partial}{\partial x_i}\left(r^{2k}\right)$ (also in (2.7)) to obtain

$$\left(\frac{d^2}{dr^2} + \frac{d-1}{r}\frac{d}{dr}\right)\left(r^{2k}\right)g(\mathbf{x}) + 4kr^{2k-2}\sum_{i=1}^{d} x_i\frac{\partial}{\partial x_i}g(\mathbf{x}) + r^{2k}\Delta g(\mathbf{x}).$$

We now compute the first term. For the second term we use lemma 2.3. We get

$$\begin{aligned}&2k(2k+d-2)r^{2k-2}g(\mathbf{x}) + 4k(n-2k)r^{2k-2}g(\mathbf{x}) + r^{2k}\Delta g(x)\\ &= 2k(2n-2k+d-2)r^{2k-2}g(\mathbf{x}) + r^{2k}\Delta g(\mathbf{x})\end{aligned}$$

Write $C = -2k(2n-2k+d-2)$, then in total we have

$$0 = -Cr^{2k-2}g(\mathbf{x}) + r^{2k}\Delta g(\mathbf{x}) \iff g(\mathbf{x}) = \frac{1}{C}r^2\Delta g(\mathbf{x})$$

Substituting this in $F(\mathbf{x}) = r^{2k}g(\mathbf{x})$ yields $F(\mathbf{x}) = \frac{1}{C}r^{2k+2}\Delta g(\mathbf{x})$. This contradicts the maximality of k and thus we must have $F = 0$. □

Proposition 2.7. *We have*

$$\mathcal{P}_n^d = \mathcal{H}_n^d \oplus ||\mathbf{x}||^2\mathcal{P}_{n-2}^d \quad (n \geq 2) \quad \textit{and} \quad \mathcal{P}_n^d = \mathcal{H}_n^d \quad (n = 0,1). \tag{2.8}$$

For the case of $n \geq 2$, this means that we can uniquely write every element of $\mathcal{P}_n^d$ as the sum of an element of $\mathcal{H}_n^d$ and an element of $||\mathbf{x}||^2\mathcal{P}_{n-2}^d$.

Proof. For all polynomials of degree smaller or equal to one we have that the Laplacian is zero and thus $\mathcal{P}_n^d = \mathcal{H}_n^d$ if $n = 0,1$. Let $n \geq 2$, then we have $\mathcal{H}_n^d, ||\mathbf{x}||^2\mathcal{P}_{n-2}^d \subseteq \mathcal{P}_n^d$. Now lemma 2.6 implies that $\mathcal{H}_n^d \cap ||\mathbf{x}||^2\mathcal{P}_{n-2}^d = \{0\}$, so we have $\dim(\mathcal{P}_n^d) \geq \dim(\mathcal{H}_n^d) + \dim(||\mathbf{x}||^2\mathcal{P}_{n-2}^d)$. To show equality it remains to prove $\dim(\mathcal{P}_n^d) \leq \dim(\mathcal{H}_n^d) + \dim(||x||^2\mathcal{P}_{n-2}^d)$.
Indeed we have

$$\dim(\mathcal{P}_n^d) = \dim(\mathcal{H}_n^d) + \dim(\Delta(\mathcal{P}_n^d)) \leq \dim(\mathcal{H}_n^d) + \dim(\mathcal{P}_{n-2}^d) = \dim(\mathcal{H}_n^d) + \dim(||\mathbf{x}||^2\mathcal{P}_{n-2}^d).$$

The first equality comes from the fact that for a linear map $\phi : V \to W$, we have $\dim(V) = \dim(\ker\phi) + \dim(\operatorname{im}\phi)$. Recall that $\ker\phi$ are all elements of V that are mapped to zero and that $\operatorname{im}\phi$ are all element of W that are of the form $\phi(v)$ for some $v \in V$. Now notice that $\Delta : \mathcal{P}_n^d \to \mathcal{P}_{n-2}^d$ is a linear map with $\ker\Delta = \mathcal{H}_n^d$ and $\operatorname{im}\Delta = \Delta(\mathcal{P}_n^d)$. The second inequality follows because $\Delta(\mathcal{P}_n^d) \subset \mathcal{P}_{n-2}^d$. We have the last equality because there is a bijection $\mathcal{P}_{n-2}^d \to ||\mathbf{x}||^2\mathcal{P}_{n-2}^d$ given by $f \mapsto ||x||^2 f$, thus their dimensions are equal. We conclude

$$\dim(\mathcal{P}_n^d) = \dim(\mathcal{H}_n^d) + \dim(||\mathbf{x}||^2\mathcal{P}_{n-2}^d),$$

which implies the desired result. □

A corollary about the dimension of $\mathcal{H}_n^d$ that follows directly from proposition 2.7 is:

Corollary 2.8. *For the dimension of $\mathcal{H}_n^d$ we have*

$$\dim\mathcal{H}_n^d = \dim\mathcal{P}_n^d - \dim\mathcal{P}_{n-2}^d \quad (n \geq 2) \quad \textit{and} \quad \dim\mathcal{H}_n^d = \dim\mathcal{P}_n^d \quad (n = 0,1) \tag{2.9}$$

We can now use this corollary to explicitly compute the dimension of $\mathcal{H}_n^d$. Using equation (2.3) we see that for $d \geq 2$ and $n \geq 1$,

$$\begin{aligned}
\dim\mathcal{H}_n^d = \dim\mathcal{P}_n^d - \dim\mathcal{P}_{n-2}^d &= \binom{n+d-1}{d-1} - \binom{n+d-3}{d-1} = \frac{(n+d-1)!}{(d-1)!n!} - \frac{(n+d-3)!}{(d-1)!(n-2)!} \\
&= \frac{(n+d-1)!(n-2)! - (n+d-3)!\,n!}{n!(n-2)!(d-1)!} \\
&= \frac{(n+d-1)(n+d-2)(n+d-3)!(n-2)! - (n+d-3)!\,n(n-1)(n-2)!}{n!(n-2)!(d-1)!} \\
&= \frac{(d^2+2nd-2n-3d+2)(n+d-3)!}{n!(d-1)(d-2)!} = \frac{(d-1)(2n+d-2)(n+d-3)!}{n!(d-1)(d-2)!} \\
&= \frac{(2n+d-2)(n+d-3)!}{n!(d-2)!}.
\end{aligned}$$

Now still for $d \geq 2$, note that for $n = 0$, we must have $f(r\mathbf{x}) = r^0 f(\mathbf{x}) = f(\mathbf{x})$, which only holds for constant functions. Thus $\dim \mathcal{H}_0^d = 1$.
For $d = 1$, the Laplacian reduces to the second derivative. And a homogeneous polynomial of degree n has the form $f(x) = x^n$. We see that $\Delta f = 0$ only holds for $n = 0,1$, so $\dim \mathcal{H}_n^1 = 1$ if $n = 0,1$ and $\dim \mathcal{H}_n^1 = 0$ if $n \geq 2$.
Next, we give some examples of harmonic homogeneous polynomials in $\mathcal{H}_n^d$.

Example 2.9.

1. For $d = n = 2$ we can easily solve $\Delta f = 0$. In this case f has the form $a_1 x_1^2 + a_2 x_2^2 + a_3 x_1 x_2$ and calculating the Laplacian and setting equal to zero yield $2a_1 + 2a_2 = 0$ which is equivalent to $a_2 = -a_1$. Substituting this back into the polynomial gives $a_1 x_1^2 - a_1 x_2^2 + a_3 x_1 x_2 = a_1(x_1^2 - x_2^2) + a_3 x_1 x_2$. Thus all polynomials are of the form $\mathcal{H}_2^2 = \{\, a(x_1^2 - x_2^2) + b x_1 x_2 \mid a, b \in \mathbb{C}\}$.

2. For $d = 2$ we have that any polynomial of the form $(x_1 + i x_2)^n$ belongs to $\mathcal{H}_n^2$. Note that $\frac{\partial^2}{\partial x_1^2}((x_1 + i x_2)^n) = n(n-1)(x_1 + i x_2)^{n-2}$ and $\frac{\partial^2}{\partial x_2^2}((x_1 + i x_2)^n) = -n(n-1)(x_1 + i x_2)^{n-2}$, because we multiply by i twice when using the chain rule.

3. For $d = 3$ and a fixed $\theta \in \mathbb{R}$, polynomials of the form $(i x_1 \cos\theta + i x_2 \sin\theta + x_3)^n$ belong to $\mathcal{H}_n^3$. To see this, observe that

$$\frac{\partial^2 f}{\partial x_1^2} = -n(n-1)\cos^2\theta (i x_1 \cos\theta + i x_2 \sin\theta + x_3)^{n-2},$$
$$\frac{\partial^2 f}{\partial x_2^2} = -n(n-1)\sin^2\theta (i x_1 \cos\theta + i x_2 \sin\theta + x_3)^{n-2},$$
$$\frac{\partial^2 f}{\partial x_3^2} = n(n-2)(i x_1 \cos\theta + i x_2 \sin\theta + x_3)^{n-2},$$

where we have written $f(x_1, x_2, x_3) = (i x_1 \cos\theta + i x_2 \sin\theta + x_3)^n$. So we get

$$\Delta f(x_1, x_2, x_3) = (-(\cos^2\theta + \sin^2\theta) + 1)\, n(n-1)(i x_1 \cos\theta + i x_2 \sin\theta + x_3)^{n-2}.$$

Noting that $-(\cos^2\theta + \sin^2\theta) + 1 = 0$ yields the result.

Note that for these functions, as seen in the examples, we can have complex coefficients. However, we do still require real-valued variables.

2.3. Spherical harmonics

We are now ready to introduce the space of spherical harmonics. By applying $f(r\mathbf{x}) = r^n f(\mathbf{x})$ to the functions in $\mathcal{H}_n$ we obtain the bijection $f \mapsto f|_{S^{d-1}}$. We call $f|_{S^{d-1}}$ a spherical harmonic of degree n on S^{d-1}. We denote the space of all spherical harmonics of degree n on S^{d-1} by $\mathcal{Y}_n^d$. Because of the bijection, we have

$$\dim(\mathcal{Y}_n^d) = \dim(\mathcal{H}_n^d),$$

so the dimensions are the same as in equation (2.9). Thus, to obtain spherical harmonics we have to restrict homogeneous harmonic polynomials to the unit sphere.

Example 2.10. Take the polynomial of the form $(x_1 + i x_2)^n$, we saw in example 2.9 that this is a homogeneous harmonic. Now in polar coordinates, for $\mathbf{x} \in S^1$ (the unit circle in this case), we have $(x_1, x_2)^T = (\cos\theta, \sin\theta)^T$ and the restriction of $(x_1 + i x_2)^n$ to the unit circle is

$$(\cos\theta + i\,\sin\theta)^n = e^{in\theta} = \cos(n\theta) + i\,\sin(n\theta),$$

which is a spherical harmonic of degree n. In addition, the real and imaginary parts are also a spherical harmonic, since for $f(\mathbf{x}) = g(\mathbf{x}) + ih(\mathbf{x})$,

$$0 = \Delta f(\mathbf{x}) = \Delta g(\mathbf{x}) + i\Delta h(\mathbf{x}) \implies \Delta g(\mathbf{x}) = \Delta h(\mathbf{x}) = 0.$$

Thus, $\cos(n\theta)$ and $\sin(n\theta)$ are also elements of $\mathcal{Y}_n^2$.

To deeper analyse spherical harmonics, we note that all spherical harmonics are elements of $L^2(S^{d-1})$, the space of square integrable functions defined on S^{d-1}. To see this, note that clearly all polynomials are square integrable. Furthermore, we can use the Lebesgue measure on $\mathbb{R}^d$ to define a surface measure on S^{d-1}, which we denote by σ. For example, this is determined by the property

$$\int_{\mathbb{R}^d} f(\mathbf{y})\, d\mathbf{y} = \int_{r=0}^{\infty} \int_{\mathbf{x}\in S^{d-1}} f(r\mathbf{x}) r^{d-1} d\sigma(\mathbf{x}) dr, \tag{2.10}$$

for all integrable functions f. Intuitively this property comes from the fact that when the radius of a sphere increases, the surface scales with r^{d-1}.
Now we can also define an inner product on $L^2(S^{d-1})$ by

$$\langle f, g\rangle := \frac{1}{\sigma(S^{d-1})} \int_{S^{d-1}} f(\mathbf{x})\overline{g(\mathbf{x})}\, d\sigma(\mathbf{x}), \tag{2.11}$$

where $\sigma\left(S^{d-1}\right)$ is the total surface area of the unit sphere in $\mathbb{R}^d$. We can make this explicit using the the gamma function (A.5):

$$\sigma\left(S^{d-1}\right) = \frac{2\pi^{d/2}}{\Gamma\left(\frac{d}{2}\right)} = \begin{cases} \frac{2\pi^{d/2}}{(\frac{d}{2}-1)!}, & d \text{ even} \\ \frac{\pi^{d/2}\cdot 2^{\frac{1}{2}d+\frac{1}{2}}}{\sqrt{\pi}(d-2)!!}, & d \text{ odd} \end{cases},$$

where we used the two properties from result A.5. Note that $n!! = n(n-2)\cdots 1$. We normalize by $\sigma\left(S^{d-1}\right)$, since this simplifies many formulas involving the inner product. Using this inner product, we can show orthogonality of spherical harmonics.

Theorem 2.11. *If $h_n \in \mathcal{H}_n^d, h_m \in \mathcal{H}_m^d$ and $n \neq m$, then $\langle h_n, h_m\rangle = 0$*

Proof. Without loss of generality we may assume h_n, h_m to be real-valued, since we can this apply this result to complex-valued functions by taking real and imaginary parts. Now by Green's first identity (A.2) we have

$$\int_{||\mathbf{x}||\le 1} \nabla h_n \cdot \nabla h_m \, d\mathbf{x} + \int_{||\mathbf{x}||\le 1} h_n \Delta h_m \, d\mathbf{x} = \int_{S^{d-1}} h_n \nabla h_m \cdot \mathbf{n}(\mathbf{x}) \, d\sigma, \tag{2.12}$$

$$\int_{||\mathbf{x}||\le 1} \nabla h_m \cdot \nabla h_n \, d\mathbf{x} + \int_{||\mathbf{x}||\le 1} h_m \Delta h_n \, d\mathbf{x} = \int_{S^{d-1}} h_m \nabla h_n \cdot \mathbf{n}(\mathbf{x}) \, d\sigma. \tag{2.13}$$

Subtracting (2.12) and (2.13) and noting that $\Delta h_n = \Delta h_m = 0$ yields

$$0 = \int_{||x||\le 1} (h_n \Delta h_m - h_m \Delta h_n)\, dx = \int_{S^{d-1}} (h_n \nabla h_m \cdot \mathbf{n}(\mathbf{x}) - h_m \nabla h_n \cdot \mathbf{n}(\mathbf{x}))\, d\sigma. \tag{2.14}$$

Now note that every point $\mathbf{x} \in S^{d-1}$ is perpendicular to the surface of S^{d-1}, so we have $\mathbf{n}(\mathbf{x}) = \mathbf{x}$ for all $\mathbf{x}$. By lemma 2.3 we obtain

$$\nabla h_m \cdot \mathbf{n}(\mathbf{x}) = \nabla h_m \cdot \mathbf{x} = \sum_{j=1}^{d} \frac{\partial f(\mathbf{x})}{\partial x_i} x_j = m f(\mathbf{x}),$$

and in the same way

$$\nabla h_n \cdot \mathbf{n}(\mathbf{x}) = n f(\mathbf{x}).$$

Substituting this into (2.14) yields

$$0 = \int_{S^{d-1}} (h_n m h_m - h_m n h_n)\, d\sigma = (m-n) \int_{S^{d-1}} h_n h_m d\sigma. \qquad \square$$

The theorem above proves that spherical harmonics are orthogonal in $L^2(S^{d-1})$ and is used to show that spherical harmonics form an orthonormal basis for $L^2(S^{d-1})$. We won't discuss the norm here, but we will return to this in chapter 3 for the case $d = 3$.

2.4. Zonal spherical harmonics

Zonal functions are functions that are invariant under rotation about a certain axis, meaning that rotating the argument of the function around this axis will not change the value of the function. To define zonal functions, we first look at the stabiliser (see A.8) of $e_1 = (1,0,...,0)$ in $O(d)$, i.e. all $T \in O(d)$ such that $Te_1 = e_1$. This is easily seen to be the following set:

$$S(d-1) = \left\{ \begin{pmatrix} 1 & 0 \\ 0 & T_1 \end{pmatrix} \middle| \; T_1 \in O(d-1) \right\}. \tag{2.15}$$

We note here that we do not necessarily have to choose e_1, we can fix any axis. In this section we fix e_1. We follow with the definition of a zonal function.

Definition 2.12. *A function f on S^{d-1} is called zonal if*

$$T \cdot f = f \quad \forall\ T \in S(d-1).$$

Since we have a bijection between $\mathcal{H}_n^d$ and $\mathcal{Y}_n^d$, we can search for zonal functions in $\mathcal{H}_n^d$ and restrict them to the unit sphere. For this we first have the following lemma for zonal functions in $\mathcal{P}_n^d$.

Lemma 2.13. *Let $f \in \mathcal{P}_n^d$. Then f is zonal if and only if, for certain coefficients c_i,*

$$f(x) = \sum_{i=0}^{\lfloor \frac{n}{2} \rfloor} c_i x_1^{n-2i} \left(x_2^2 + \cdots + x_d^2\right)^i, \tag{2.16}$$

where $\lfloor \frac{n}{2} \rfloor$ is $\frac{n}{2}$ rounded down to an integer.

Proof. First suppose f is of the form (2.16), then we see that f has maximum degree n. Furthermore, for $T \in S(d-1)$ we have that $T^{-1}\mathbf{x} = T^T\mathbf{x}$ does not change the first element of $\mathbf{x}$. The rest of the vector is determined by $T_1^{-1}(x_2,...,x_d)^T = T_1^T(x_2,...,x_d)^T$. Since $T_1 \in O(d-1)$ this will not change the length of $(x_2,...,x_d)^T$. So noting that f is dependent on powers of x_1 and $||(x_2,..,x_d)||^{2i}$, we can conclude that $T \cdot f(\mathbf{x}) = f(T^T\mathbf{x}) = f(\mathbf{x})$ for all $\mathbf{x}$.
Conversely, suppose $f \in \mathcal{P}_n^d$ is zonal. Then for certain homogeneous polynomials f_k of degree k in $x_2,...,x_d$, we can write

$$f(x) = \sum_{k=0}^{n} x_1^{n-k} f_k(x_2,...,x_d),$$

by factoring out x^{n-k} for every $k \in \mathbb{N} \cup \{0\}$. Now note that $S(d-1)$ contains the reflection

$$R : (x_1, x_2, ..., x_d) \mapsto (x_1, -x_2, ..., -x_d).$$

Since f is zonal, we have $R \cdot f = f$, so

$$\sum_{k=0}^{n} x_1^{n-k} f_k(x_2,...,x_d) = \sum_{k=0}^{n} x_1^{n-k} f_k(-x_2,...,-x_d) = \sum_{k=0}^{n} x_1^{n-k} (-1)^k f_k(x_2,...,x_d),$$

where we used homogeneity in the last equality. For odd k we thus see

$$x_1^{n-k} f_k(x_2,...,x_d) = -x_1^{n-k} f_k(x_2,...,x_d),$$

since we do not necessarily have $x_1 = 0$, we must have $f_k = 0$ for odd k. We can write

$$f(x) = \sum_{i=0}^{\lfloor \frac{n}{2} \rfloor} x_1^{n-2i} f_{2i}(x_2, ..., x_d).$$

Now for every $(x_1, x_2, ..., x_d)$ we can construct a rotation $R_{\mathbf{x}} \in S(d-1)$ given by

$$R_{\mathbf{x}} : (x_1, x_2, ..., x_d) \mapsto \left(x_1, \sqrt{x_2^2 + \cdots + x_d^2}, 0, ..., 0\right).$$

For this take

$$R_{\mathbf{x}} = \begin{pmatrix} 1 & 0 \\ 0 & T_1 \end{pmatrix},$$

with a $T_1 \in O(d-1)$ such that $T_1(x_2, ..., x_d)^T = \left(\sqrt{x_2^2 + \cdots + x_d^2}, 0, \ldots, 0\right)$. With this map, again since f is zonal, we have

$$f(x) = \sum_{i=0}^{\lfloor n/2 \rfloor} x_1^{n-2i} f_{2i}(x_2, \ldots, x_d) = \sum_{i=0}^{\lfloor n/2 \rfloor} x_1^{n-2i} f_{2i}\left(\sqrt{x_2^2 + \cdots + x_d^2}, 0, \ldots, 0\right).$$

Since now every f_{2i} only depends on the first variable and since they are homogeneous of degree $2i$, we must have

$$\sum_{i=0}^{\lfloor n/2 \rfloor} x_1^{n-2i} f_{2i}\left(\sqrt{x_2^2 + \cdots + x_d^2}, 0, \ldots, 0\right) = \sum_{i=0}^{\lfloor n/2 \rfloor} c_i x_1^{n-2i} (x_2^2 + \cdots + x_d^2)^i,$$

for certain coefficients c_i. □

The next proposition implies that all zonal harmonic homogeneous polynomials of the same degree are multiples of each other.

Proposition 2.14. *The space of zonal functions in $\mathcal{H}_n^d$ has dimension 1.*

Proof. By lemma 2.13 we know that a function $f \in \mathcal{P}_n^d$ is zonal in $\mathcal{H}_n^d$ if and only if f has the form (2.16) and satisfies $\Delta f = 0$, thus we check when $\Delta f = 0$ holds. For this write $\rho := \sqrt{x_2^2 + \cdots + x_d^2}$, then as in the proof lemma 2.6, we use that Δ acts on a function only depending on ρ as $\frac{d^2}{d\rho^2} + \frac{d-2}{\rho}\frac{d}{d\rho}$ (where we now have $d-2$, because we start at x_2). Applying Δ to f we see

$$\Delta f = \frac{\partial^2 f}{\partial x_1^2} + \left(\frac{\partial^2 f}{\partial x_2^2} + \cdots + \frac{\partial^2 f}{\partial x_d^2}\right) = \frac{\partial^2 f}{\partial x_1^2} + \frac{d^2 f}{d\rho^2} + \frac{d-2}{\rho}\frac{df}{d\rho}.$$

Computing this yields

$$\begin{aligned}\Delta f &= \sum_{i=0}^{\lfloor \frac{n}{2} \rfloor} c_i \left((n-2i)(n-2i-1)x_1^{n-2i-2}\rho^{2i} + x_1^{n-2i}\left(\frac{d^2}{d\rho^2}\left(\rho^{2i}\right) + \frac{d-2}{\rho}\frac{d}{d\rho}\left(\rho^{2i}\right)\right)\right) \\ &= \sum_{i=0}^{\lfloor \frac{n}{2} \rfloor} c_i \left((n-2i)(n-2i-1)x_1^{n-2i-2}\rho^{2i} + 2i(2i+d-3)x_1^{n-2i}\rho^{2i-2}\right) = 0.\end{aligned}$$

Note that $2i(2i+d-3)x_1^{n-2i}\rho^{2i-2} = 0$ for $i = 0$ and that $(n-2i)(n-2i-1)x_1^{n-2i-2}\rho^{2i} = 0$ for $i = \lfloor \frac{n}{2} \rfloor$ ($n-2i = 0$ for even n, $n-2i-1 = 0$ for odd n). With this we can rewrite the above expression into

$$\sum_{i=1}^{\lfloor \frac{n}{2} \rfloor} \left((n-2i+2)(n-2i+1)c_{i-1} + 2i(2i+d-3)c_i\right) x_1^{n-2i}\rho^{2i-2} = 0,$$

where we shifted the index. From this we deduce that

$$c_i = -\frac{(n-2i+2)(n-2i+1)}{2i(2i+d-3)}\, c_{i-1} \qquad \left(i = 1, \dots, \lfloor \tfrac{n}{2} \rfloor\right).$$

We can conclude that all coefficients are dependent on the choice of c_0, i.e. all zonal functions in $\mathcal{H}_n^d$ are determined by multiples of c_0. □

To find the explicit form of these functions, we follow with three results. For this we first give a parametrisation of the unit sphere in $\mathbb{R}^d$, which is used in these results. We want to parametrise $\mathbf{x} = (x_1, ..., x_d)^T \in S^{d-1}$ in terms of x_1. This can be done by first noting that for $\mathbf{x} \in S^{d-1}$,

$$\mathbf{x} = x_1(1,0,...,0)^T + (0, x_2, ..., x_d)^T = x_1 e_1 + (0, x_2, ..., x_d)^T.$$

Now we want to rewrite $(0, x_2, ..., x_d)^T$ in terms of a vector with length one. So we write $(0, x_2, ..., x_d)^T = a\mathbf{x}'$, where $\mathbf{x}'$ is a vector with length one and $x_1 = 0$. To determine a we solve:

$$1 = ||\mathbf{x}||^2 = ||x_1 e_1 + a\mathbf{x}'||^2 = x_1^2 + a^2,$$

so $a = \sqrt{1 - x_1^2}$. Now write $t := x_1$ and $S_0^{d-1} := \{\mathbf{x} \in S^{d-1} \mid x_1 = 0\}$, then we obtain the parametrisation

$$\mathbf{x} = te_1 + \sqrt{1-t^2}\mathbf{x}' \qquad t \in [-1,1],\ \mathbf{x}' \in S_0^{d-1}.$$

Proposition 2.15. *Let $d \geq 3$. Define S_0^{d-1} as above and let σ' be the surface measure on S_0^{d-1}. Then, for all $f \in C(S^{d-1})$,*

$$\int_{S^{d-1}} f\, d\sigma = \int_{\mathbf{x}' \in S_0^{d-1}} \int_{t=-1}^{1} f\left(te_1 + \sqrt{1-t^2}\mathbf{x}'\right)(1-t^2)^{\frac{1}{2}d - \frac{3}{2}}\, dt\, d\sigma'(\mathbf{x}'). \tag{2.17}$$

Proof. A vector $\mathbf{y} = (y_1, ... y_d)^T$, can be decomposed into $y_1 e_1 = (y_1, 0, ..., 0)^T$ and $\mathbf{y}' = (0, y_2, ..., y_d)^T$. Now for functions g with $g \neq 0$ outside a compact set we can write

$$\int_{\mathbb{R}^d} g(\mathbf{y})\, d\mathbf{y} = \int_{\mathbb{R}^{d-1}} \int_{y_1=-\infty}^{\infty} g(y_1 e_1 + (0, y_2, .., y_d))\, dy_1 d(y_2, ..., y_d)$$

Now we can apply (2.10) to the outer integral to obtain

$$\int_{\mathbf{x}' \in S_0^{d-1}} \int_{\rho=0}^{\infty} \int_{y_1=-\infty}^{\infty} g(y_1 e_1 + \rho\mathbf{x}')\, \rho^{d-2}\, dy_1\, d\rho\, d\sigma'(\mathbf{x}').$$

We use a change of variable, let $y_1 = rt$ and $\rho = r\sqrt{1-t^2}$. Then the Jacobian is

$$\begin{vmatrix} \frac{\partial y_1}{\partial t} & \frac{\partial y_1}{\partial r} \\ \frac{\partial \rho}{\partial t} & \frac{\partial \rho}{\partial r} \end{vmatrix} = \begin{vmatrix} r & t \\ -\frac{rt}{\sqrt{1-t^2}} & \sqrt{1-t^2} \end{vmatrix} = r\sqrt{1-t^2} + \frac{rt^2}{\sqrt{1-t^2}} = r(1-t^2)^{-\frac{1}{2}}.$$

For the new bounds note that $y_1^2 = r^2 t^2$ and $\rho^2 = r^2(1-t^2)$. Thus

$$y_1^2 + \rho^2 = r^2(t^2 + 1 - t^2) = r^2 \implies r = \sqrt{y_1^2 + \rho^2},$$

and

$$t = \frac{y_1}{r} = \frac{y_1}{\sqrt{y_1^2 + \rho^2}}.$$

Since r is the root of a positive number, we have $r \in [0,\infty)$. For t we see

$$\lim_{y_1\to\pm\infty} t = \lim_{y_1\to\pm\infty} \frac{y_1}{\sqrt{y_1^2+\rho^2}} = \lim_{y_1\to\pm\infty} \frac{y_1}{|y_1|\sqrt{1+\rho^2/y_1^2}} = \pm 1,$$

so $t \in (-1,1)$. We obtain

$$\begin{aligned}\int_{\mathbf{x}'\in S_0^{d-1}} \int_{t=-1}^{1} \int_{r=0}^{\infty} g\left(rte_1 + r\sqrt{1-t^2}\mathbf{x}'\right)\left(r\sqrt{1-t^2}\right)^{d-2}\left(r(1-t^2)^{-\frac{1}{2}}\right) dr\, dt\, d\sigma'(\mathbf{x}') \\ = \int_{\mathbf{x}'\in S_0^{d-1}} \int_{t=-1}^{1} \int_{r=0}^{\infty} g\left(r\left(te_1 + \sqrt{1-t^2}\mathbf{x}'\right)\right)(1-t^2)^{\frac{1}{2}d-\frac{3}{2}} r^{d-1}\, dr\, dt\, d\sigma'(\mathbf{x}').\end{aligned}$$

We are interested in the integral over the unit sphere, so we assume that g has the form $g(\mathbf{y}) = h(r)f(\mathbf{x})$, for some function h. Now comparing what we found above to the rewriting in (2.10) yields

$$\begin{aligned}\int_{r=0}^{\infty}\int_{\mathbf{x}\in S^{d-1}} f(\mathbf{x})h(r)r^{d-1} d\sigma(\mathbf{x})dr \\ = \int_{\mathbf{x}'\in S_0^{d-1}} \int_{t=-1}^{1} \int_{r=0}^{\infty} f\left(te_1 + \sqrt{1-t^2}\mathbf{x}'\right)(1-t^2)^{\frac{1}{2}d-\frac{3}{2}} h(r) r^{d-1}\, dr\, dt\, d\sigma'(\mathbf{x}').\end{aligned}$$

Since g has a compact support, the integral over r is bounded and so we can divide it out to obtain the desired result. □

As a corollary, we obtain

Corollary 2.16. *Let $d \geq 2$ and let $f \in C(S^{d-1})$ be zonal. Then*

$$\frac{1}{\sigma(S^{d-1})}\int_{S^{d-1}} f\, d\sigma = \frac{\Gamma\left(\frac{1}{2}d\right)}{\Gamma\left(\frac{1}{2}d-\frac{1}{2}\right)\Gamma\left(\frac{1}{2}\right)}\int_{-1}^{1} f\left(te_1+\sqrt{1-t^2}\,e_2\right)(1-t^2)^{\frac{1}{2}d-\frac{3}{2}}\, dt, \tag{2.18}$$

where Γ is the gamma function. (One can write these gamma functions explicitly using the properties in result A.5.)

Proof. We apply proposition 2.15 to get

$$\frac{1}{\sigma(S^{d-1})}\int_{S^{d-1}} f\, d\sigma = \frac{1}{\sigma(S^{d-1})}\int_{\mathbf{x}'\in S_0^{d-1}}\int_{t=-1}^{1} f\left(te_1+\sqrt{1-t^2}\mathbf{x}'\right)(1-t^2)^{\frac{1}{2}d-\frac{3}{2}}\, dt\, d\sigma'(\mathbf{x}').$$

Since f is zonal, $f\left(te_1+\sqrt{1-t^2}\mathbf{x}'\right)$ is independent of $\mathbf{x}'$, in particular we can set $\mathbf{x}' = e_2$. We obtain

$$\begin{aligned}\frac{1}{\sigma(S^{d-1})}\int_{S^{d-1}} f\, d\sigma &= \frac{1}{\sigma(S^{d-1})}\int_{\mathbf{x}'\in S_0^{d-1}}\int_{t=-1}^{1} f\left(te_1+\sqrt{1-t^2}\,e_2\right)(1-t^2)^{\frac{1}{2}d-\frac{3}{2}}\, dt\, d\sigma'(\mathbf{x}') \\ &= \frac{\sigma'(S_0^{d-1})}{\sigma(S^{d-1})}\int_{t=-1}^{1} f\left(te_1+\sqrt{1-t^2}\,e_2\right)(1-t^2)^{\frac{1}{2}d-\frac{3}{2}}\, dt.\end{aligned}$$

Now note that we have this equality for all $f \in C(S^{d-1})$, so we can set $f = 1$. Then we see

$$\frac{1}{\sigma(S^{d-1})}\int_{S^{d-1}} 1\, d\sigma = 1 = \frac{\sigma'(S_0^{d-1})}{\sigma(S^{d-1})}\int_{t=-1}^{1} 1\cdot(1-t^2)^{\frac{1}{2}d-\frac{3}{2}}\, dt,$$

so that

$$\frac{\sigma(S^{d-1})}{\sigma'(S_0^{d-1})} = \int_{-1}^{1}(1-t^2)^{\frac{1}{2}d-\frac{3}{2}}\, dt.$$

To compute this integral, we first note that $(1-t^2)^{\frac{1}{2}d-\frac{3}{2}}$ is an even function, so we have

$$\int_{-1}^{1}(1-t^2)^{\frac{1}{2}d-\frac{3}{2}}\,dt = 2\int_{0}^{1}(1-t^2)^{\frac{1}{2}d-\frac{3}{2}}\,dt.$$

Now let $t=\sqrt{x}$, then $dt=\frac{1}{2}x^{-\frac{1}{2}}dx$ and we obtain

$$2\int_{0}^{1}(1-t^2)^{\frac{1}{2}d-\frac{3}{2}}\,dt = 2\int_{0}^{1}(1-x)^{\frac{1}{2}d-\frac{3}{2}}\cdot\frac{1}{2}x^{-\frac{1}{2}}\,dx = \int_{0}^{1}(1-x)^{(\frac{1}{2}d-\frac{1}{2})-1}\cdot x^{\frac{1}{2}-1}\,dx.$$

We recognize this form as a beta function (A.6) for which we have

$$\mathrm{B}(x_1,x_2)=\int_0^1 x^{x_1-1}(1-x)^{x_2-1}\,dx=\frac{\Gamma(x_1)\Gamma(x_2)}{\Gamma(x_1+x_2)}.$$

Thus

$$\frac{\sigma(S^{d-1})}{\sigma'(S_0^{d-1})}=\int_{-1}^{1}(1-t^2)^{\frac{1}{2}d-\frac{3}{2}}\,dt=\mathrm{B}\left(\frac{1}{2}d-\frac{1}{2},\frac{1}{2}\right)=\frac{\Gamma(\frac{1}{2}d-\frac{1}{2})\Gamma(\frac{1}{2})}{\Gamma(\frac{1}{2}d)}.$$ □

The following theorem will show that the explicit form of zonal spherical harmonics are Jacobi polynomials. There are multiple ways to define Jacobi polynomials, here we define them using Rodrigues' formula:

$$P_n^{(\alpha,\beta)}(x)=\frac{(-1)^n}{2^n n!}(1-x)^{-\alpha}(1+x)^{-\beta}\frac{d^n}{dx^n}\left((1-x)^{\alpha}(1+x)^{\beta}(1-x^2)^n\right). \tag{2.19}$$

A property of Jacobi polynomials that will be used in proving theorem is that for $n\neq\ell$ we have

$$\int_{-1}^{1}P_n^{(\alpha,\beta)}(x)P_\ell^{(\alpha,\beta)}(x)(1-x)^{\alpha}(1+x)^{\beta}\,dx=0, \tag{2.20}$$

whenever $\alpha,\beta>-1$.

Theorem 2.17. *Let $f\in\mathcal{H}_n^d$. Then f is zonal if and only if, for the restriction of f to S^{d-1},*

$$f(\mathbf{x})=f\left(te_1+\sqrt{1-t^2}\,\mathbf{x}'\right)=CP_n^{(\frac{1}{2}d-\frac{3}{2},\frac{1}{2}d-\frac{3}{2})}(t),\qquad t\in[-1,1],\mathbf{x}'\in S_0^{d-1},C\in\mathbb{C}. \tag{2.21}$$

Here $P_n^{(\frac{1}{2}d-\frac{3}{2},\frac{1}{2}d-\frac{3}{2})}(t)$ is a Jacobi polynomials with $\alpha=\beta=\frac{1}{2}d-\frac{3}{2}$

Proof. For each n choose a nonzero real-valued zonal function $\phi_n\in\mathcal{H}_n^d$. By lemma 2.13 and the fact that $x_2^2+\cdots+x_d^2=1-x_1^2=1-t^2$, we have constants c_i such that

$$\phi_n\left(te_1+\sqrt{1-t^2}\,x'\right)=\sum_{i=0}^{\lfloor\frac{n}{2}\rfloor}c_i\,t^{n-2i}(1-t^2)^i.$$

Here we see that ϕ_n only depends on t and is a polynomial with maximum degree n, we denote this polynomial in t by p_n. Now by theorem 2.11 and corollary 2.16, for $n\neq m$, we obtain

$$0=\int_{S^{d-1}}\phi_n\phi_m d\sigma=\frac{\Gamma\left(\frac{1}{2}d\right)}{\Gamma\left(\frac{1}{2}d-\frac{1}{2}\right)\Gamma\left(\frac{1}{2}\right)}\int_{-1}^{1}p_n(t)p_m(t)(1-t^2)^{\frac{1}{2}d-\frac{3}{2}}\,dt.$$

Dividing by the constant gives

$$\int_{-1}^{1}p_n(t)p_m(t)(1-t)^{\frac{1}{2}d-\frac{3}{2}}(1+t)^{\frac{1}{2}d-\frac{3}{2}}\,dt=0.$$

Hence p_n is a polynomial that is orthogonal with respect to the weight $(1-t)^{\frac{1}{2}d-\frac{3}{2}}(1+t)^{\frac{1}{2}d-\frac{3}{2}}$. It can be shown that this is exactly a Jacobi polynomial with $\alpha = \beta = \frac{1}{2}d - \frac{3}{2}$ as defined above. For this, take a sequence $\left(p_n\right)_{n=0}^{\infty}$ of polynomials, with the degree of p_n equal to n. We assume them to be orthogonal, but by dividing through the norm we can assume $\langle p_n, p_m\rangle = \delta_{nm}$. In the same way let $\left(q_n\right)_{n=0}^{\infty}$ be a different sequence of polynomials with the same properties. Now suppose we have a polynomial $q = \sum_{k=0}^{m} c_k q_k$ with $m < n$. Then

$$\langle q_n, q\rangle = \left\langle q_n, \sum_{k=0}^{m} c_k q_k \right\rangle = \sum_{k=0}^{m} c_k \langle q_n, q_k\rangle = 0, \tag{2.22}$$

where we used orthonormality. Now we can write $q_n = \sum_{k=0}^{n} c_k p_k$ so that

$$\langle q_n, p_m\rangle = \left\langle \sum_{k=0}^{n} c_k p_k, p_m \right\rangle = \sum_{k=0}^{n} c_k \langle p_k, p_m\rangle = c_m.$$

But now by (2.22) we see that $c_m = \langle q_n, p_m\rangle = 0$ if $m < n$. We conclude that $q_n = c_n p_n$. □

3

The Laplace Equation in $\mathbb{R}^3$

In many applications such as 3D representation and angular momentum, we turn to spherical harmonics in three dimensions. In this chapter we deduce an explicit formula for spherical harmonics in three dimensions by solving Laplace's equation directly using spherical coordinates. Furthermore, we compute the norm of the spherical harmonics to normalize these functions. This chapter is based on notes by Haber[7] and a book by Boas[2].

3.1. The Laplace operator

As defined in (2.6), the Laplacian operator in Cartesian coordinates in three dimensions is given by

$$\Delta f(x,y,z) = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} + \frac{\partial^2 f}{\partial z^2}. \tag{3.1}$$

However, in three dimensions it might not be too surprising that we turn to spherical coordinates. Recall that spherical coordinates are given by

$$x = r\sin\theta\cos\phi, \quad y = r\sin\theta\sin\phi, \quad z = r\cos\theta, \tag{3.2}$$

where $r \in [0,\infty)$, $\theta \in [0,\pi]$, $\phi \in [0,2\pi)$. To express the Laplacian in spherical coordinates, we need to compute $\Delta f(r,\theta,\phi)$. For this we have to first express r,θ,ϕ in terms of x,y,z, which can be done as follows

$$r = \sqrt{x^2+y^2+z^2}, \quad \theta = \cos^{-1}\left(\frac{z}{\sqrt{x^2+y^2+z^2}}\right), \quad \phi = \text{sign}(y)\cdot\cos^{-1}\left(\frac{x}{\sqrt{x^2+y^2}}\right), \tag{3.3}$$

where sign(y) is the sign of y. We can now use to chain rule to find the first derivative of $f(r,\theta,\phi)$ with respect to x:

$$\frac{\partial f}{\partial x} = \frac{\partial f}{\partial r}\frac{\partial r}{\partial x} + \frac{\partial f}{\partial \theta}\frac{\partial \theta}{\partial x} + \frac{\partial f}{\partial \phi}\frac{\partial \phi}{\partial x}.$$

In the same way we can compute the first derivatives with respect to y and z. However, these derivatives get complicated fast, so we will not further compute these here. For the full derivation, see for example [12]. The Laplacian in spherical coordinates is given by

$$\Delta f(r,\theta,\phi) = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial f}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta\frac{\partial f}{\partial \theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2 f}{\partial \phi^2}. \tag{3.4}$$

3.2. Solving the Laplace equation

Now that we have introduced the Laplacian in spherical coordinates, we can solve the Laplace equation:

$$\Delta f(r,\theta,\phi) = 0. \tag{3.5}$$

To solve this equation, we will start by assuming that the solution has the form

$$f(r,\theta,\phi) = R(r)\Theta(\theta)\Phi(\phi). \tag{3.6}$$

Not all solution are of this form, however, any solution can by approximated as a linear combination of (3.6). We will touch more one this later. Substituting (3.6) into (3.4) yields

$$\begin{aligned}
\Delta f(r,\theta,\phi) &= \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial f}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial f}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2 f}{\partial\phi^2} \\
&= \frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR(r)\Theta(\theta)\Phi(\phi)}{dr}\right) + \frac{1}{r^2\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{dR(r)\Theta(\theta)\Phi(\phi)}{d\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{d^2R(r)\Theta(\theta)\Phi(\phi)}{d\phi^2} \\
&= \frac{\Theta(\theta)\Phi(\phi)}{r^2}\frac{d}{dr}\left(r^2\frac{dR(r)}{dr}\right) + \frac{R(r)\Phi(\phi)}{r^2\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta(\theta)}{d\theta}\right) + \frac{R(r)\Theta(\theta)}{r^2\sin^2\theta}\frac{d^2\Phi(\phi)}{d\phi^2} = 0 \\
&\implies \frac{\sin^2\theta}{R(r)}\frac{d}{dr}\left(r^2\frac{dR(r)}{dr}\right) + \frac{\sin\theta}{\Theta(\theta)}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta(\theta)}{d\theta}\right) + \frac{1}{\Phi(\phi)}\frac{d^2\Phi(\phi)}{d\phi^2} = 0,
\end{aligned}$$

where in the last step we multiplied by $\frac{r^2\sin^2(\theta)}{R(r)\Theta(\theta)\Phi(\phi)}$. We can rewrite this into

$$-\frac{1}{\Phi(\phi)}\frac{d^2\Phi(\phi)}{d\phi^2} = \frac{\sin^2\theta}{R(r)}\frac{d}{dr}\left(r^2\frac{dR(r)}{dr}\right) + \frac{\sin\theta}{\Theta(\theta)}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta(\theta)}{d\theta}\right). \tag{3.7}$$

Now note that the left-hand side of the equation only depends on ϕ, while the right-hand side only depends on r and θ. Thus the equation can only be satisfied if both sides equal a constant. For the left hand side, for a constant $C \in \mathbb{R}$, we obtain

$$-\frac{1}{\Phi(\phi)}\frac{d^2\Phi(\phi)}{d\phi^2} = C \iff \frac{d^2\Phi(\phi)}{d\phi^2} = -C\Phi(\phi) \iff \frac{d^2\Phi(\phi)}{d\phi^2} + C\Phi(\phi) = 0. \tag{3.8}$$

This is a second-order homogeneous linear ODE and recall that this has solutions of the form $e^{r\phi}$, where r is given by solving

$$r^2 + C = 0 \iff r = \begin{cases} \pm i\sqrt{C}, & \text{if } C \geq 0 \\ \pm\sqrt{C}, & \text{if } C < 0 \end{cases}.$$

This gives solutions of the form $e^{\pm i\sqrt{C}\phi}$. However, note that ϕ is a periodic variable with period 2π, so we need $\Phi(\phi + 2\phi) = \Phi(\phi)$. For $e^{\pm\sqrt{C}\phi}$ we need

$$e^{\pm\sqrt{C}\phi}e^{\pm\sqrt{C}\cdot 2\pi} = e^{\pm\sqrt{C}\phi}.$$

This equality holds whenever $e^{i\sqrt{C}2\pi} = 1$, which in turn holds when $2\pi C = 2\pi m^2$ for some $m \in \mathbb{Z}$. Thus we need $C = m^2$ and we can write all solutions as

$$\Phi(\phi) = ae^{im\phi} \quad a \in \mathbb{C},\ m \in \mathbb{Z}.$$

Now with equation (3.8) and $C = m^2$, we can write

$$-\frac{1}{\Phi(\phi)}\frac{d^2\Phi(\phi)}{d\phi^2} = m^2. \tag{3.9}$$

Substituting this back into equation (3.7), we obtain

$$m^2 = \frac{\sin^2\theta}{R(r)}\frac{d}{dr}\left(r^2\frac{dR(r)}{dr}\right) + \frac{\sin\theta}{\Theta(\theta)}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta(\theta)}{d\theta}\right),$$

which can be rewritten into

$$\frac{1}{R(r)}\frac{d}{dr}\left(r^2\frac{dR(r)}{dr}\right) = -\frac{1}{\Theta(\theta)\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta(\theta)}{d\theta}\right) + \frac{m^2}{\sin^2\theta}. \tag{3.10}$$

Now we have the left hand side only depending on r, while the right hand side only depends on θ. So as before, for a constant $D \in \mathbb{C}$, we can set

$$\frac{1}{R(r)}\frac{d}{dr}\left(r^2\frac{dR(r)}{dr}\right) = D \iff \frac{d}{dr}\left(r^2\frac{dR(r)}{dr}\right) - DR(r) = 0.$$

In this case we choose $D = \ell(\ell+1)$, $\ell \in \mathbb{N}\cup\{0\}$, for reasons that will become clear later. Working out the derivative using the product rule yields

$$r^2\frac{d^2R(r)}{dr^2} + 2r\frac{dR(r)}{dr} - \ell(\ell+1)R(r) = 0. \tag{3.11}$$

We recognize this as Euler's equation, which has solutions of the form $R(r) = r^s$ for some $s \in \mathbb{R}$. To determine s, we substitute this solution into equation (3.11). We obtain

$$\begin{aligned} 0 &= r^2 s(s-1)r^{s-2} + 2rsr^{s-1} - \ell(\ell+1)r^2 \\ &= s(s-1)r^s + 2sr^s - \ell(\ell+1)r^s \\ &= r^s(s(s-1) + 2s - \ell(\ell+1)). \end{aligned}$$

Since $r^s > 0$, we get

$$s(s-1) + 2s - \ell(\ell+1) = 0 \iff s(s+1) = \ell(\ell+1) \iff s = \ell \ \vee\ s = -\ell - 1.$$

Thus the general solution is

$$R(r) = pr^\ell + qr^{-\ell-1}, \quad p, q \in \mathbb{C}. \tag{3.12}$$

Finally, with equation (3.10) and $D = \ell(\ell+1)$ we obtain

$$\ell(\ell+1) = -\frac{1}{\Theta(\theta)\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta(\theta)}{d\theta}\right) + \frac{m^2}{\sin^2\theta},$$

which is equivalent to

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta(\theta)}{d\theta}\right) + \left(\ell(\ell+1) - \frac{m^2}{\sin^2\theta}\right)\Theta(\theta) = 0. \tag{3.13}$$

To solve for $\Theta(\theta)$, we make a change of variables. For this let $x = \cos\theta$ and $y(x) = \Theta(\theta)$. Then using the chain rule, we see

$$\frac{d\Theta(\theta)}{d\theta} = \frac{dy}{dx}\frac{dx}{d\theta} = \frac{dy}{dx}(-\sin\theta) = -\sin\theta\frac{dy}{dx},$$

and thus

$$\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta(\theta)}{d\theta}\right) = \frac{d}{d\theta}\left(-\sin^2\theta\frac{dy}{dx}\right) = -2\sin\theta\cos\theta\frac{dy}{dx} - \sin^2\theta\frac{d^2y}{dx^2}\frac{dx}{d\theta}.$$

We can substitute this into the first term of equation (3.13) to obtain

$$-2\cos\theta\frac{dy}{dx} + \sin^2\theta\frac{d^2y}{dx^2} = 0.$$

Finally, with $\cos\theta = x$ and $\sin^2\theta = 1-\cos^2\theta = 1-x^2$, we see

$$(1-x^2)\frac{d^2y}{dx^2} - 2x\frac{dy}{dx} + \left(\ell(\ell+1) - \frac{m^2}{1-x^2}\right)y = 0. \tag{3.14}$$

We chose $D = \ell(\ell+1)$ since the equation we have now obtained is a special type of equation, namely the associated Legendre equation. A note here is that this choice of D is more a physical reason than a mathematical one, since other choices of D can still yield mathematically feasible solutions. However, since we will look at a physical application in chapter 4, we choose $D = \ell(\ell+1)$ here. Now we can show that the function

$$P_\ell^m(x) = \frac{(-1)^m}{2^\ell \ell!}(1-x^2)^{m/2}\frac{d^{\ell+m}}{dx^{\ell+m}}(x^2-1)^\ell, \qquad |m| \le \ell, \tag{3.15}$$

solves this equation. The derivation of this will not be shown here, for reference see chapter 12 of [2].
Putting everything we found together, we have that the general solution of the Laplacian in spherical coordinates is:

$$R(r)\Theta(\theta)\Phi(\phi) = (pr^\ell + qr^{-\ell-1})(P_\ell^m(\cos\theta))ae^{im\phi}, \tag{3.16}$$

where $a, p, q \in \mathbb{C}$ and $\ell \in \mathbb{N}\cup\{0\}$, $m \in \mathbb{Z}$ with $|m| \le \ell$.

3.3. Orthonormality

On the the unit sphere, we have $r = 1$, and so (3.16) above reduces to

$$R(1)\Theta(\theta)\Phi(\phi) = (p+q)(P_\ell^m(\cos\theta))ae^{im\phi}$$

By absorbing all constants into a single constant, we can write the general solution as

$$\tilde{Y}_\ell^m(\theta,\phi) = CP_\ell^m(\cos\theta)e^{im\phi}, \qquad C \in \mathbb{C}, \tag{3.17}$$

which is the collection of not yet normalised spherical harmonics in three dimensions. Note that for $m = 0$, the exponential is equal to one, meaning the functions become invariant to rotation about the z-axis. In other words, for $m = 0$ we have the collection of zonal spherical harmonics in three dimensions. This can also be seen by setting $d = 3$ in theorem 2.17, then we see $P_\ell^{(0,0)} = P_\ell^0$.

In theorem 2.11, we showed that spherical harmonics are orthogonal to each other (see proposition B.1 for an elementary proof of this for $d = 3$). So what remains is finding the constant C such that $\tilde{Y}_\ell^m(\theta,\phi)$ is normalised. For this, we compute $\langle \tilde{Y}_\ell^m, \tilde{Y}_\ell^m\rangle$. Now note that the inner product in (2.11) is defined for Cartesian coordinates. However, since $\tilde{Y}_\ell^m$ is defined in spherical coordinates, we transform the integral. The Jacobian of this transformation is $r^2\sin\theta$, so with $r = 1$ we see

$$\begin{aligned}\langle \tilde{Y}_\ell^m, \tilde{Y}_\ell^m\rangle &= \frac{1}{\sigma(S^2)}\int_{S^2} \tilde{Y}_\ell^m, \overline{\tilde{Y}_\ell^m}\, d\sigma = \frac{1}{4\pi}\int_0^{2\pi}\int_0^\pi P_\ell^m(\cos\theta)e^{im\phi}P_\ell^m(\cos\theta)e^{-im\phi}\sin\theta\; d\theta d\phi \\ &= \frac{1}{4\pi}\int_0^{2\pi}\int_0^\pi P_\ell^m(\cos\theta)^2\sin\theta\; d\theta d\phi = \frac{2\pi}{4\pi}\int_0^\pi P_\ell^m(\cos\theta)^2\sin\theta\; d\theta.\end{aligned}$$

Now we make a change of variables back to Cartesian coordinates with $x = \cos\theta$ and so $dx = \sin\theta\; d\theta$, which yields

$$\frac{1}{2}\int_{-1}^1 P_\ell^m(x)^2\; dx.$$

For this integral we have the following theorem.

Theorem 3.1. *For $\ell, n \in \mathbb{N}$ and $m \in \mathbb{Z}$ with $|m| \le \ell$, we have*

$$\int_{-1}^{1} P_\ell^m(x) P_n^m(x)\, dx = \delta_{\ell n} \frac{2}{2\ell+1} \frac{(\ell+m)!}{(\ell-m)!},$$

where

$$\delta_{\ell n} = \begin{cases} 1, & \text{if } \ell = n \\ 0, & \text{if } \ell \neq n \end{cases}.$$

Proof. Without loss of generality, for now we assume $\ell \ge n$. Write

$$I_{\ell n}^m = \int_{-1}^{1} P_\ell^m(x) P_n^m(x)\, dx = \frac{1}{2^{n+\ell}\, n!\, \ell!} \int_{-1}^{1} \left((1-x^2)^m \frac{d^{n+m}}{dx^{n+m}} (x^2-1)^n \right) \left(\frac{d^{\ell+m}}{dx^{\ell+m}} (x^2-1)^\ell \right) dx.$$

We now integrate by parts $\ell + m$ times

$$\int_{-1}^{1} u(x) v'(x) dx = [u(x)v(x)]_{-1}^{1} - \int_{-1}^{1} u'(x) v(x) dx,$$

with $u(x) = (1-x^2)^m \frac{d^{n+m}}{dx^{n+m}} (x^2-1)^n$ and $v'(x) = \frac{d^{\ell+m}}{dx^{\ell+m}} (x^2-1)^\ell$. Then note that for the first m integrations by parts, $u(x)$ in $[u(x)v(x)]_{-1}^{1}$ contains the term $(1-x^2)$, since this term is 0 at the endpoints, $[u(x)v(x)]_{-1}^{1}$ vanishes. For the remaining ℓ integrations, $v(x)$ contains the term (x^2-1). Thus we obtain

$$I_{\ell n}^m = \frac{(-1)^{\ell+m}}{2^{n+\ell}\, n!\, \ell!} \int_{-1}^{1} (x^2-1)^\ell \frac{d^{\ell+m}}{dx^{\ell+m}} \left((1-x^2)^m \frac{d^{n+m}}{dx^{n+m}} (x^2-1)^n \right) dx.$$

Applying Leibniz's rule (A.3) to the second term in the integral yields

$$\frac{d^{\ell+m}}{dx^{\ell+m}} \left((1-x^2)^m \frac{d^{n+m}}{dx^{n+m}} (x^2-1)^n \right) = \sum_{k=0}^{\ell+m} \binom{\ell+m}{k} \frac{d^k}{dx^k} (1-x^2)^m \frac{d^{\ell+n+2m-k}}{dx^{\ell+n+2m-k}} (x^2-1)^n.$$

For the first derivative in the sum we see that this is non-zero for $r \le 2m$, since $(1-x^2)^m$ is a polynomial of degree $2m$. Recall that $m \le \ell$, so we do reach $2m$ in the sum. The second derivative is non-zero when $\ell + n + 2m - k \le 2n$ or equivalently $r \ge \ell - n + 2m$. We thus have that $I_{\ell n}^m \neq 0$ when

$$\ell - n + 2m \le r \le 2m \implies \ell - n + 2m \le 2m \iff \ell \le n,$$

but by assumption we have $\ell \ge n$ and so we must have $\ell = n$. Substituting this in the bound for r we also have $r = 2m$. Putting this all into $I_{\ell n}^m$ gives

$$I_{n\ell}^m = \delta_{\ell n} (-1)^\ell \frac{(-1)^{\ell+m}}{2^{2\ell} (\ell!)^2} \binom{\ell+m}{2m} \int_{-1}^{1} (x^2-1)^\ell \frac{d^{2m}}{dx^{2m}} (1-x^2)^m \frac{d^{2\ell}}{dx^{2\ell}} (1-x^2)^\ell\, dx,$$

where we also factored out $(-1)^\ell$. To evaluate the two derivatives within the integral, we apply the binomial theorem (A.4) to expand $(1-x^2)^r$:

$$(1-x^2)^r = \sum_{i=0}^{r} \binom{r}{i} \cdot 1^r \cdot \left((-x^2)^{r-i} \right) = \sum_{i=0}^{r} \binom{r}{i} (-1)^{r-i} x^{2(r-i)}.$$

After differentiating this $2r$-times we see that only the first term of the sum is non-zero, so

$$\frac{d^{2r}}{dx^{2r}} (1-x^2)^r = \frac{d^{2r}}{dx^{2r}} \left(\binom{r}{0} (-1)^r x^{2r} \right) = (-1)^r (2r)!.$$

Thus we see

$$\begin{aligned}
I_{n\ell}^{m} &= \delta_{\ell n}(-1)^{\ell}\frac{(-1)^{\ell+m}}{2^{2\ell}(\ell!)^2}\binom{\ell+m}{2m}\int_{-1}^{1}(x^2-1)^{\ell}\,(-1)^m(2m)!(-1)^{\ell}(2\ell)!\,dx\\
&= \delta_{\ell n}(-1)^{\ell}\frac{1}{2^{2\ell}(\ell!)^2}\frac{(\ell+m)!}{(2m)!(\ell-m)!}\int_{-1}^{1}(x^2-1)^{\ell}(2m)!(2\ell)!\,dx\\
&= \delta_{\ell n}(-1)^{\ell}\frac{(2\ell)!}{2^{2\ell}(\ell!)^2}\frac{(\ell+m)!}{(\ell-m)!}\int_{-1}^{1}(x^2-1)^{\ell}\,dx.
\end{aligned}$$

We evaluate

$$\int_{-1}^{1}(x^2-1)^{\ell}\,dx$$

by setting $x=\cos\theta$, then

$$\int_{-1}^{1}(x^2-1)^{\ell}\,dx=(-1)^{\ell}\int_{-1}^{1}(1-x^2)^{\ell}\,dx=(-1)^{\ell+1}\int_{\pi}^{0}\sin^{2\ell+1}(\theta)\;d\theta=(-1)^{\ell}\int_{0}^{\pi}\sin^{2\ell+1}(\theta)\;d\theta.$$

To compute this integral note that

$$\begin{aligned}
\frac{d}{d\theta}\left(\sin^{n-1}\theta\cos\theta\right) &= (n-1)\sin^{n-2}\theta\cos^2\theta-\sin^{n-1}\theta\sin\theta\\
&= (n-1)\sin^{n-2}\theta(1-\sin^2\theta)\theta-\sin^{n-1}\theta\sin\theta\\
&= (n-1)\sin^{n-2}\theta-(n-1)\sin^{n}\theta-\sin^{n}\theta\\
&= (n-1)\sin^{n-2}\theta-n\sin^{n}\theta.
\end{aligned}$$

Integrating both sides and rearranging yields

$$\int_{0}^{\pi}\sin^{n}\theta\,d\theta=\frac{1}{n}\left[-\sin^{n-1}\theta\cos\theta\right]_0^{\pi}+\frac{n-1}{n}\int_{0}^{\pi}\sin^{n-2}\theta\,d\theta=\frac{n-1}{n}\int_{0}^{\pi}\sin^{n-2}\theta\,d\theta,$$

where we used that $\sin\theta=0$ for $\theta=0,\pi$. Applying this we get

$$(-1)^{\ell}\int_{0}^{\pi}\sin^{2\ell+1}(\theta)=(-1)^{\ell}\frac{2\ell}{2\ell+1}\int_{0}^{\pi}\sin^{2\ell-1}\theta\;d\theta=(-1)^{\ell}\frac{2\ell}{2\ell+1}\int_{0}^{\pi}\sin^{2\ell+1}\theta\sin^{-2}\theta\;d\theta.$$

By changing back to x we obtain

$$\int_{-1}^{1}(x^2-1)^{\ell}\,dx=-\frac{2\ell}{2\ell+1}\int_{-1}^{1}(x^2-1)^{\ell-1}dx.$$

Applying this recursively we get

$$\int_{-1}^{1}(x^2-1)^{\ell}\,dx=(-1)^{\ell}\left(\frac{2\ell}{2\ell+1}\cdot\frac{2(\ell-1)}{2\ell-1}\cdot\frac{2(\ell-2)}{2\ell-3}\cdots\frac{2}{3}\right)\int_{-1}^{1}dx,$$

and for the right expression we see

$$\frac{2\ell}{2\ell+1}\cdot\frac{2(\ell-1)}{2\ell-1}\cdot\frac{2(\ell-2)}{2\ell-3}\cdots\frac{2}{3}=\frac{2^{\ell}\,\ell!}{(2\ell+1)(2\ell-1)(2\ell-3)\cdots3}=\frac{2^{\ell}\,\ell!}{\frac{(2\ell+1)!}{2^{\ell}\,\ell!}}=\frac{2^{2\ell}(\ell!)^2}{(2\ell+1)!},$$

so that

$$\int_{-1}^{1}(x^2-1)^{\ell}\,dx=(-1)^{\ell}\frac{2^{2\ell+1}(\ell!)^2}{(2\ell+1)!}.$$

We can thus conclude that

$$\begin{aligned}\int_{-1}^{1} P_\ell^m(x)P_n^m(x)\ dx &= \delta_{\ell n}(-1)^\ell \frac{(2\ell)!}{2^{2\ell}(\ell!)^2}\frac{(\ell+m)!}{(\ell-m)!}\int_{-1}^{1}(x^2-1)^\ell\ dx \\ &= \delta_{\ell n}(-1)^\ell \frac{(2\ell)!}{2^{2\ell}(\ell!)^2}\frac{(\ell+m)!}{(\ell-m)!}\cdot(-1)^\ell\frac{2^{2\ell+1}(\ell!)^2}{(2\ell+1)!} \\ &= \delta_{\ell n}\frac{2}{2\ell+1}\frac{(\ell+m)!}{(\ell-m)!}. \end{aligned}$$

□

With this we obtain the normalisation factor of $\tilde{Y}_\ell^m(\theta,\phi)$, since

$$\langle \tilde{Y}_\ell^m, \tilde{Y}_\ell^m\rangle = \frac{1}{2}\int_{-1}^{1} P_\ell^m(x)^2\ dx = -\frac{1}{2}\frac{2}{2\ell+1}\frac{(\ell+m)!}{(\ell-m)!} = -\frac{1}{2\ell+1}\frac{(\ell+m)!}{(\ell-m)!}.$$

Thus, setting setting $C = \sqrt{-2\ell+1\frac{(\ell-m)!}{(\ell+m)!}}$ in (3.17), we have

$$Y_\ell^m(\theta,\phi) = \sqrt{-(2\ell+1)\frac{(\ell-m)!}{(\ell+m)!}}P_\ell^m(\cos\theta)e^{im\phi},$$

which satisfies

$$\langle Y_\ell^m, Y_\ell^m\rangle = 1.$$

A final important property of the spherical harmonics in $\mathbb{R}^d$, which we state without proof here, is that the spherical harmonics form a complete basis for $L^2(S^2)$. This implies that any function $f(\theta,\phi) \in L^2(S^2)$ can be written as

$$f(\theta,\phi) = \sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell} a_{\ell m} Y_\ell^m(\theta,\phi). \tag{3.18}$$

This property will be useful in the application we will discuss in the following chapter.

4

Angular Momentum

In this section, we will turn to an application of spherical harmonics: angular momentum. We start by introducing the notion of operators in quantum mechanics. After introducing the angular momentum operators, we will show that spherical harmonics are the eigenfunctions of these operators and why discuss this is useful. The mathematics in this chapter are clearly explained in a book by Hall[8]. For the physical side, refer to this introductory book on quantum mechanics[6].

4.1. Preliminaries

4.1.1. Operators in $\mathbb{R}$

In quantum mechanics, the position of a particle is determined using a wave function. A wave function, denoted by ψ, assigns a probability to the location of a particle. Let us first assume that we have a particle moving along the real number line. Then for such a particle, we have a wave function $\psi : \mathbb{R} \to \mathbb{C}$. ψ depends on the position x and time t, but for now we assume time independence, so we write $\psi(x)$. Now the probability density of the location of a particle is given by $|\psi(x)|^2$, where $|\psi(x)|^2 = \psi(x)\overline{\psi(x)}$ is the modulus squared. Thus we have that the probability that a particle is within some Borel set $A \subseteq \mathbb{R}$ is

$$\int_A |\psi(x)|^2 dx.$$

Since $|\psi(x)|^2$ is a density, we also have

$$\int_{\mathbb{R}} |\psi(x)|^2 dx = 1.$$

Furthermore, we can define the expectation of the position:

$$\langle x \rangle := \int_{\mathbb{R}} x|\psi(x)|^2 dx, \tag{4.1}$$

assuming that this integral is convergent. Now you might wonder how we can interpret this expectation. As you might know, when measuring a quantum particle, the wave function describing it collapses as it will be located at one point. This means that the expectation of the position is not the average of different measurement of the same quantum particles. Rather, we can see it as averaging the measurements of different quantum particles all in the state ψ.

In quantum mechanics expectations of various quantities are expressed in terms of operators and the inner product on the relevant space, in this case $L^2(\mathbb{R})$. On $L^2(\mathbb{R})$[1] we can define the position operator X by

$$(X\psi)(x) := x\psi(x).$$

[1]Not for all $\psi \in L^2(\mathbb{R})$, we will touch on this later.

We can now write (4.1) as

$$\langle x\rangle = \langle X\psi, \psi\rangle_{\mathbb{R}},$$

where the inner product is defined as

$$\langle f, g\rangle_{\mathbb{R}} := \int_{\mathbb{R}} f(x)\overline{g(x)}dx.$$

Besides the position, another property of particles is momentum. In classical mechanics, momentum relates velocity and mass by multiplying the two. So to introduce momentum in quantum mechanics, we need some information on the velocity. For this, we introduce time-dependence and write $\psi(x,t)$. Now the velocity is the derivative of the position, so we want to find an expression for

$$\frac{d}{dt}\langle x\rangle(t) = \frac{\partial}{\partial t}\int_{\mathbb{R}} x|\psi(x,t)|^2\, dx.$$

Note that this is the derivative of the *expectation* of the position, so it will not give deterministic information on the velocity, but it will help us derive the momentum operator. In this derivation we do leave out some mathematical details. To find this quantity, we will first find an expression for $\frac{\partial}{\partial t}|\psi(x,t)|^2$. For this we introduce the Schrödinger equation:

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t) + V(x,t)\psi(x,t), \tag{4.2}$$

where m is the mass of a particle, $\hbar = \frac{h}{2\pi}$, with h being Plank's constant and $V : \mathbb{R}\times\mathbb{R}_{\geq 0} \to \mathbb{R}$ is the potential that represents the environment in which the particle exists. Now rewriting the Schrödinger equation gives

$$\frac{\partial}{\partial t}\psi(x,t) = \frac{i\hbar}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t) - \frac{i}{\hbar}V(x,t)\psi(x,t). \tag{4.3}$$

Taking the complex conjugate of this equation yields

$$\frac{\partial}{\partial t}\overline{\psi(x,t)} = -\frac{i\hbar}{2m}\frac{\partial^2}{\partial x^2}\overline{\psi(x,t)} + \frac{i}{\hbar}V(x,t)\overline{\psi(x,t)}. \tag{4.4}$$

Now using the product rule we find

$$\frac{\partial}{\partial t}|\psi(x,t)|^2 = \frac{\partial}{\partial t}\left(\psi(x,t)\overline{\psi(x,t)}\right) = \psi(x,t)\frac{\partial}{\partial t}\overline{\psi(x,t)} + \overline{\psi(x,t)}\frac{\partial}{\partial t}\psi(x,t).$$

By substituting in (4.3) and (4.4) we obtain

$$\begin{aligned}\frac{\partial}{\partial t}|\psi(x,t)|^2 &= \frac{i\hbar}{2m}\left(-\psi(x,t)\left(\frac{\partial^2}{\partial x^2}\overline{\psi(x,t)} + \frac{i}{\hbar}V(x,t)\overline{\psi(x,t)}\right) + \overline{\psi(x,t)}\left(\frac{\partial^2}{\partial x^2}\psi(x,t) + \frac{i}{\hbar}V(x,t)\psi(x,t)\right)\right)\\ &= \frac{i\hbar}{2m}\left(-\psi(x,t)\frac{\partial^2}{\partial x^2}\overline{\psi(x,t)} + \overline{\psi(x,t)}\frac{\partial^2}{\partial x^2}\psi(x,t)\right)\\ &= \frac{i\hbar}{2m}\frac{\partial}{\partial x}\left(-\psi(x,t)\frac{\partial}{\partial x}\overline{\psi(x,t)} + \overline{\psi(x,t)}\frac{\partial}{\partial x}\psi(x,t)\right),\end{aligned}$$

where in the last step we again used the product rule. Finally, we find

$$\begin{aligned}
\frac{d}{dt}\langle x\rangle(t) &= \frac{\partial}{\partial t}\int_{\mathbb{R}} x|\psi(x,t)|^2 dx = \int_{\mathbb{R}} x\frac{\partial}{\partial t}|\psi(x,t)|^2 dx \\
&= \frac{i\hbar}{2m}\int_{\mathbb{R}} x\frac{\partial}{\partial x}\left(-\psi(x,t)\frac{\partial}{\partial x}\overline{\psi(x,t)} + \overline{\psi(x,t)}\frac{\partial}{\partial x}\psi(x,t)\right) dx \\
&= \frac{i\hbar}{2m}\left[x\left(-\psi(x,t)\frac{\partial}{\partial x}\overline{\psi(x,t)} + \overline{\psi(x,t)}\frac{\partial}{\partial x}\psi(x,t)\right)\right]_{x=-\infty}^{\infty} \\
&\qquad - \frac{i\hbar}{2m}\int_{\mathbb{R}} -\psi(x,t)\frac{\partial}{\partial x}\overline{\psi(x,t)} + \overline{\psi(x,t)}\frac{\partial}{\partial x}\psi(x,t) dx \\
&= -\frac{i\hbar}{2m}\int_{\mathbb{R}} -\psi(x,t)\frac{\partial}{\partial x}\overline{\psi(x,t)} + \overline{\psi(x,t)}\frac{\partial}{\partial x}\psi(x,t) dx \\
&= \frac{i\hbar}{2m}\int_{\mathbb{R}} \psi(x,t)\frac{\partial}{\partial x}\overline{\psi(x,t)} dx - \frac{i\hbar}{2m}\int_{\mathbb{R}} \overline{\psi(x,t)}\frac{\partial}{\partial x}\psi(x,t) dx \\
&= \frac{i\hbar}{2m}\left(\left[\psi(x,t)\overline{\psi(x,t)}\right]_{x=-\infty}^{\infty} - \int_{\mathbb{R}} \overline{\psi(x,t)}\frac{\partial}{\partial x}\psi(x,t) dx\right) - \frac{i\hbar}{2m}\int_{\mathbb{R}} \overline{\psi(x,t)}\frac{\partial}{\partial x}\psi(x,t) dx \\
&= -\frac{i\hbar}{m}\int_{\mathbb{R}} \overline{\psi(x,t)}\frac{\partial}{\partial x}\psi(x,t) dx,
\end{aligned}$$

where we used integration by parts twice and the fact that ψ goes to zero at $\pm\infty$ (This does not hold for all $\psi \in L^2(\mathbb{R})$, but we will choose an appropriate set of function later). Now as in the classical case, we multiply this by m and obtain a momentum operator. We see

$$-i\hbar\int_{\mathbb{R}} \overline{\psi(x,t)}\frac{\partial}{\partial x}\psi(x,t) dx = \langle -i\hbar\frac{\partial}{\partial x}\psi, \psi\rangle_{\mathbb{R}}.$$

Thus, we define the momentum operator by

$$(P\psi)(x) := -i\hbar\frac{d\psi(x)}{dx},$$

where we dropped the time-dependence again.
Note that for a function $\psi(x) \in L^2(\mathbb{R})$, both $(X\psi)(x)$ and $(P\psi)(x)$ could fail to be in $L^2(\mathbb{R})$ again. How to deal with this properly is beyond the scope of this report. Therefore, we will work with Schwartz functions. These functions are infinity differentiable, bounded, and rapidly decreasing.
An important property of these two operators is that they do not commute, i.e. $X(P\psi(x)) \neq P(X\psi(x))$. We see this as follows

$$X(P\psi(x)) = X\left(-i\hbar\frac{d\psi(x)}{dx}\right) = -i\hbar x\frac{d\psi(x)}{dx}, \tag{4.5}$$

$$P(X\psi(x)) = P\left(x\psi(x)\right) = -i\hbar\frac{d}{dx}(x\psi(x)) = -i\hbar\left(\psi(x) + x\frac{d\psi(x)}{dx}\right) \tag{4.6}$$

However, X and P do satisfy the canonical commutation relation which is defined as follows.

Definition 4.1. *For two operators A and B, the canonical commutation relation is*

$$[A,B] = AB - BA.$$

Now we have the following relation between X and P.

Proposition 4.2. *The position and momentum operators X and P satisfy the relation*

$$[X,P] = i\hbar I.$$

Proof. Using (4.5) and (4.6) we get

$$\begin{aligned} P(X\psi(x)) &= -i\hbar\left(\psi(x) + x\frac{d\psi(x)}{dx}\right) \\ &= -i\hbar\psi(x) - i\hbar x\frac{d\psi(x)}{dx} \\ &= i\hbar\psi(x) + X(P(\psi(x)), \end{aligned}$$

from which the result follows. □

4.1.2. Operators in $\mathbb{R}^3$

We can now generalise what we found in section 4.1.1 to $\mathbb{R}^3$. Note that we can also generalise to $\mathbb{R}^d$, but we only need three dimensions for angular momentum.
For the position and momentum operators, instead of one operator, we have 3 operators given by

$$\begin{aligned} X_j\psi(\mathbf{x}) &= x_j\psi(\mathbf{x}), \\ P_j\psi(\mathbf{x}) &= -i\hbar\frac{\partial\psi(\mathbf{x})}{\partial x_j}, \end{aligned}$$

for $j = 1,2,3$. As a generalisation of proposition 4.2, we have the following result.

Proposition 4.3. *The position and momentum operators in* $\mathbb{R}^3$ *satisfy*

$$[X_j, X_k] = 0, \tag{4.7}$$

$$[P_j, P_k] = 0, \tag{4.8}$$

$$[X_j, P_k] = i\hbar\delta_{jk}I \tag{4.9}$$

for all $1 \le j,k \le 3$.

Proof. For the first two results, we easily see

$$\begin{aligned} [X_j, X_k]\psi(\mathbf{x}) &= x_jx_k\psi(\mathbf{x}) - x_kx_j\psi(\mathbf{x}) = 0, \\ [P_j, P_k]\psi(x) &= -i\hbar\frac{\partial}{\partial x_j}\frac{\partial}{\partial x_k}\psi(\mathbf{x}) + i\hbar\frac{\partial}{\partial x_k}\frac{\partial}{\partial x_j}\psi(\mathbf{x}) = 0. \end{aligned}$$

For the last result we have

$$\begin{aligned} \frac{1}{i\hbar}[X_j, P_k]\psi(\mathbf{x}) &= \frac{1}{i\hbar}\left(X_j(P_k\psi(\mathbf{x})) - P_k(X_j\psi(\mathbf{x}))\right) \\ &= \frac{1}{i\hbar}\left(-i\hbar x_j\frac{\partial\psi(\mathbf{x})}{\partial x_k} + i\hbar\frac{\partial}{\partial x_k}(x_j\psi(\mathbf{x}))\right). \end{aligned}$$

Computing this for $j = k$ and $j \neq k$ yields the result. □

4.2. Angular momentum operators

Now that we have introduced the notion of operators, we can introduce the angular momentum operator. In classical mechanics the angular momentum is calculated as $\mathbf{r} \times \mathbf{p}$, the cross product of a particles position vector $\mathbf{r}$ and momentum vector $\mathbf{p} = m\mathbf{v}$. In quantum mechanics angular momentum is similarly defined as the cross product between the position and momentum operators. We define the operators on the unit sphere. Writing x, y, z for x_1, x_2, x_3, we have that the angular momentum is defined by

$$\mathbf{J} := \begin{pmatrix} X \\ Y \\ Z \end{pmatrix} \times \begin{pmatrix} P_x \\ P_y \\ P_z \end{pmatrix} = \begin{pmatrix} YP_z - ZP_y \\ ZP_x - XP_z \\ XP_x - YP_x \end{pmatrix} = -i\hbar \begin{pmatrix} y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y} \\ z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z} \\ x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x} \end{pmatrix},$$

where in calculating the cross product we used the commutation relation (4.9) from proposition 4.3. Thus, for each direction we have the following operators:

$$J_x = -i\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right), \quad J_y = -i\hbar\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right), \quad J_z = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right).$$

To find the relation between these operators and the spherical harmonics found in chapter 3, we make a transformation to spherical coordinates and call the new operators L_x, L_y, L_z. This transformation is an elementary (but long) calculation, so we will not show it here. We see that

$$L_x = i\hbar\left(\sin\phi\frac{\partial}{\partial\theta} + \frac{\cos\phi}{\tan\theta}\frac{\partial}{\partial\phi}\right), \quad L_y = i\hbar\left(-\cos\phi\frac{\partial}{\partial\theta} + \frac{\sin\phi}{\tan\theta}\frac{\partial}{\partial\phi}\right), \quad L_z = -i\hbar\frac{\partial}{\partial\phi},$$

are the angular momentum operator in spherical coordinates. Note that these do not depend on r as we assumed that we are working on the unit sphere. Besides the directional operators for angular momentum, we can also look at the total angular momentum, which is written as

$$L^2 = L_x^2 + L_y^2 + L_z^2,$$

which is equal to

$$L^2 = -\hbar^2\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right). \tag{4.10}$$

For these operators, we have the following commutation relations:

$$[L_x, L_y] = i\hbar L_z, \quad [L_y, L_z] = i\hbar L_x, \quad [L_z, L_x] = i\hbar L_y, \tag{4.11}$$

and

$$[L^2, L_x] = 0, \quad [L^2, L_y] = 0, \quad [L^2, L_z] = 0. \tag{4.12}$$

By symmetry, it suffices to show $[L_x, L_y] = i\hbar L_z$ and $[L^2, L_x] = 0$. We show these relations using J_x, J_y, J_z. We first compute

$$[J_x, J_y] = [XP_z - ZP_y,\ ZP_x - XP_z].$$

By expanding this and using $[A+B, C] = [A, C] + [B, C]$ we get

$$[YP_z, ZP_x] - [YP_z, XP_z] - [ZP_y, ZP_x] + [ZP_y, XP_z].$$

For the products, we use

$$[AB, CD] = A[B, C]D + AC[B, D] + [A, C]DB + C[A, D]B,$$

and apply this to every term. This yields

$$\begin{aligned}
[YP_z, ZP_x] &= Y[P_z, Z]P_x + YZ[P_z, P_x] + [Y, Z]P_zP_x + Z[Y, P_x]P_z \\
&= Y(-i\hbar)P_x + 0 + 0 + Z(0)P_z = -i\hbar YP_x, \\
[YP_z, XP_z] &= Y[P_z, X]P_z + YX[P_z, P_z] + [Y, X]P_zP_z + X[Y, P_z]P_z \\
&= Y(0)P_z + 0 + 0 + X(i\hbar)P_z = i\hbar XP_z, \\
[ZP_y, ZP_x] &= Z[P_y, Z]P_x + ZZ[P_y, P_x] + [Z, Z]P_yP_x + Z[Z, P_x]P_y \\
&= Z(0)P_x + 0 + 0 + Z(0)P_y = 0, \\
[ZP_y, XP_z] &= Z[P_y, X]P_z + ZX[P_y, P_z] + [Z, X]P_yP_z + X[Z, P_z]P_y \\
&= Z(-i\hbar)P_z + 0 + 0 + X(i\hbar)P_y = -i\hbar ZP_z + i\hbar XP_y.
\end{aligned}$$

By combining the terms we obtain

$$
\begin{aligned}
[J_x, J_y] &= (-i\hbar YP_x) - (i\hbar XP_z) - 0 + (-i\hbar ZP_z + i\hbar XP_y) \\
&= i\hbar(XP_y - YP_x) \\
&= i\hbar J_z.
\end{aligned}
$$

For $[J^2, J_x]$ we see

$$[J^2, J_x] = [J_x^2 + J_y^2 + J_z^2, J_x] = [J_x^2, J_x] + [J_y^2, J_x] + [J_z^2, J_x].$$

First, $[J_x^2, J_x] = 0$ because J_x commutes with itself. For the second and third term, we use $[A^2, B] = A[A,B] + [A,B]A$ and we obtain

$$[J_y^2, J_x] = J_y[J_y, J_x] + [J_y, J_x]J_y.$$

Using $[J_y, J_x] = -i\hbar J_z$ we get

$$[J_y^2, J_x] = J_y(-i\hbar J_z) + (-i\hbar J_z)J_y = -i\hbar(J_yJ_z + J_zJ_y).$$

Finally, we have

$$[J_z^2, J_x] = J_z[J_z, J_x] + [J_z, J_x]J_z = J_z(i\hbar J_y) + (i\hbar J_y)J_z = i\hbar(J_zJ_y + J_yJ_z),$$

now using $[J_z, J_x] = i\hbar J_y$, We conclude

$$[J^2, J_x] = 0 + \big(-i\hbar(J_yJ_z + J_zJ_y)\big) + \big(i\hbar(J_zJ_y + J_yJ_z)\big) = 0.$$

With this we can also conclude that $[L_x, L_y] = i\hbar L_z$ and $[L^2, L_x] = 0$. Furthermore, we have that they are linear operators. Indeed for $f, g \in L^2(\mathbb{R}^3)$ and $a, b \in \mathbb{C}$, we see

$$
\begin{aligned}
L_x(af+bg) &= i\hbar\left(\sin\phi\frac{\partial}{\partial\theta}(af+bg) + \frac{\cos\phi}{\tan\theta}\frac{\partial}{\partial\phi}(af+bg)\right) \\
&= i\hbar\left(\sin\phi\left(a\frac{\partial f}{\partial\theta} + b\frac{\partial g}{\partial\theta}\right) + \frac{\cos\phi}{\tan\theta}\left(a\frac{\partial f}{\partial\phi} + b\frac{\partial g}{\partial\phi}\right)\right) \\
&= aL_x(f) + bL_x(g), \\
L_y(af+bg) &= i\hbar\left(-\cos\phi\frac{\partial}{\partial\theta}(af+bg) + \frac{\sin\phi}{\tan\theta}\frac{\partial}{\partial\phi}(af+bg)\right) \\
&= i\hbar\left(-\cos\phi\left(a\frac{\partial f}{\partial\theta} + b\frac{\partial g}{\partial\theta}\right) + \frac{\sin\phi}{\tan\theta}\left(a\frac{\partial f}{\partial\phi} + b\frac{\partial g}{\partial\phi}\right)\right) \\
&= aL_y(f) + bL_y(g), \\
L_z(af+bg) &= -i\hbar\frac{\partial}{\partial\phi}(af+bg) \\
&= -i\hbar\left(a\frac{\partial f}{\partial\phi} + b\frac{\partial g}{\partial\phi}\right) \\
&= aL_z(f) + bL_z(g), \\
L^2(af+bg) &= -\hbar^2\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}(af+bg)\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}(af+bg)\right) \\
&= -\hbar^2\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta(a\frac{\partial f}{\partial\theta} + b\frac{\partial g}{\partial\theta})\right) + \frac{1}{\sin^2\theta}\left(a\frac{\partial^2 f}{\partial\phi^2} + b\frac{\partial^2 g}{\partial\phi^2}\right)\right) \\
&= aL^2(f) + bL^2(g).
\end{aligned}
$$

4.3. Eigenfunctions

So far, we have seen position, momentum, and angular momentum in quantum mechanics. In this section we will show that performing calculation for particles described by a wave function of the form $\tilde{Y}_\ell^m(\theta,\phi)$ found in chapter 3 simplify a lot. For this we first define eigenfunctions.

Definition 4.4. *Let D be a linear operator and $f \neq 0$ a function. Then f is an eigenfunction of D with eigenvalue $\lambda \in \mathbb{C}$ if*

$$Df(\mathbf{x}) = \lambda f(\mathbf{x}).$$

If we now take $D = L_z$ for example, finding an eigenfunction f for this operator means that if we have a particle in the state f, we know that $L_z f = \lambda f$. This means that calculating the z-component of the angular momentum is very straightforward. So in the optimal case we want to find a function that is the eigenfunction of multiple operators. However, for a function to be the eigenfunction of multiple operators, the operators must commute on the span of a function f. To see this, suppose we have a function f such that $L_x f = \lambda f$ and $L_y f = \mu f$, then

$$[L_x, L_y]f = L_x L_y f - L_y L_x f = \mu L_x f - \lambda L_y f = \mu\lambda f - \mu\lambda f = 0.$$

Thus we need the operators to commute on the span of f. However, in (4.11) we saw that L_x and L_y do not commute, so we must chose operators that do commute. In (4.12) we saw that L^2 commutes with $L_x, L_y,$ and L_z. So we can try to find an eigenfunction for L^2 and one of the directional operators.

We will show that the eigenfunctions of L_z and L^2 are $\tilde{Y}_\ell^m(\theta,\phi) = CP_\ell^m(\cos\theta)e^{im\phi}$, as given in (3.17). For L_z we easily see that

$$L_z(\tilde{Y}(\theta,\phi)) = -i\hbar\frac{\partial}{\partial\phi}\left(CP_\ell^m(\cos\theta)e^{im\phi}\right) = -i(im)\hbar CP_\ell^m(\cos\theta)e^{im\phi} = \hbar m CP_\ell^m(\cos\theta)e^{im\phi},$$

so $Y(\theta,\phi)$ is an eigenfunction of L_z with eigenvalue $\hbar m$.

Now for L^2 notice that (4.10) is exactly the angular part of the Laplacian in spherical coordinates (3.4) multiplied by $-\hbar^2$. Recall that in (3.9) we found

$$-\frac{1}{\Phi(\phi)}\frac{d^2\Phi(\phi)}{d\phi^2} = m^2,$$

and in (3.13)

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta(\theta)}{d\theta}\right) + \left(\ell(\ell+1) - \frac{m^2}{\sin^2\theta}\right)\Theta(\theta) = 0,$$

where $\Theta(\theta)$ and $\Phi(\phi)$ are from the separation of variables in (3.6). So substituting (3.9) in (3.13) yields

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta(\theta)}{d\theta}\right) + \left(\ell(\ell+1) + \frac{1}{\Phi(\phi)\sin^2\theta}\frac{d^2\Phi(\phi)}{d\phi^2}\right)\Theta(\theta) = 0,$$

which is equivalent to

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta(\theta)\Phi(\phi)}{d\theta}\right) + \frac{1}{\sin^2\theta}\frac{d^2\Theta(\theta)\Phi(\phi)}{d\phi^2} = -\ell(\ell+1)\Theta(\theta)\Phi(\phi).$$

Now we know that this equation is satisfied by $\tilde{Y}_\ell^m(\theta,\phi) = CP_\ell^m(\cos\theta)e^{im\phi}$. So now we observe that

$$\begin{aligned}
L^2(\tilde{Y}_\ell^m(\theta,\phi)) &= -\hbar^2\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\tilde{Y}_\ell^m(\theta,\phi)\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\tilde{Y}_\ell^m(\theta,\phi)\right)\\
&= -\hbar^2\left(-\ell(\ell+1)\tilde{Y}_\ell^m(\theta,\phi)\right)\\
&= \hbar^2\ell(\ell+1))\tilde{Y}_\ell^m(\theta,\phi).
\end{aligned}$$

Thus $Y_\ell^m(\theta,\phi)$ is an eigenfunction of L^2 with eigenvalue $\hbar^2\ell(\ell+1)$.
Now these results do not only imply that calculating the properties of particles in the state $Y_\ell^m(\theta,\phi)$ can be simplified. Namely, if we use (3.18), we can decompose any function in $L^2(S^2)$ into a linear combination of spherical harmonics. In such, we can apply the results above to each individual component of the linear combination and so the spherical harmonics form a nice basis when working with angular momentum.

5

Discussion and Future Work

This report was written to provide a structured and accessible introduction to spherical harmonics. We started with rigorously introducing spherical harmonics by restricting harmonic homogeneous polynomials to the unit sphere. Using this theory we looked at zonal spherical harmonics and its properties.
The rest of the report focussed on three dimensions, where we found an explicit formula for the space of spherical harmonics and normalised these functions. With this, we turned to an application: angular momentum. Here we used spherical harmonics as a nice basis within quantum measurement.

Now obviously, there remains a lot open for further study. For example,
spherical harmonics have a deep connection with group theory, more so than discussed in this report. The lecture notes of Koornwinder[9] treat this in a lot of detail. This group theoretical aspect, which was not discussed in detail in this report, is also present in the angular momentum application from chapter 4.
Besides the abstract theory, one can also look at the numerical aspect of spherical harmonics. Efficient computation of spherical harmonic coefficients is essential in fields such as computer graphics and climate modelling. The work of Driscoll and Healy[5] on fast algorithms and recent improvements using Fibonacci grids[11] are valuable extensions.
Finally, there are many other applications like modelling Earth's gravitational potentiation[10]. Spherical harmonics are also essential in the study of the cosmic microwave background. The angular power spectrum of the cosmic microwave background is analysed using spherical harmonic decompositions, as documented in works like Dodelson's Modern Cosmology[4]. Besides these applications, one can also look at the applications mentioned in the introduction.

In short, there are endless possibilities for the use of spherical harmonics!

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A

Some Useful Results and Definitions

Theorem A.1 (Chain rule). *Let $D \subseteq \mathbb{R}^d$, and let $f : D \to \mathbb{R}$ be differentiable. Furthermore, let $E \subseteq \mathbb{R}^n$ and for each $i \in 1, ..., d$, let $u_i : E \to \mathbb{R}$ be differentiable. Then, with $u_i(\mathbf{t}) = u(t_1, ..., t_n)$, we have*

$$\frac{\partial}{\partial t_j} f(u_1, ..., u_d) = \frac{\partial f}{\partial x_1}\frac{\partial x_1}{\partial t_j} + \frac{\partial f}{\partial x_2}\frac{\partial x_2}{\partial t_j} + \cdots + \frac{\partial f}{\partial x_d}\frac{\partial x_d}{\partial t_j}, \tag{A.1}$$

for any $j = 1, ..., n$.

Theorem A.2 (Green's first identity). *Let $U \subseteq \mathbb{R}^d$. Suppose $f : U \to \mathbb{R}$ is once continuously differentiable and $g : U \to \mathbb{R}$ twice continuously differentiable. Then*

$$\int_U \nabla f \cdot \nabla g \, dV + \int_U f \, \Delta g \, dV = \int_{\partial U} f \, \nabla g \cdot \mathbf{n}(\mathbf{x}) \, dS, \tag{A.2}$$

where ∂U is the boundary of U and $\mathbf{n}$ is the outward pointing normal vector at the point $\mathbf{x}$.

Theorem A.3 (Leibniz's rule). *Let f, g be n-times differentiable. Then fg is n-times differentiable and*

$$(fg)^{(n)} = \sum_{k=0}^{n} \binom{n}{k} f^{(n-k)} g^{(k)}. \tag{A.3}$$

Theorem A.4 (Binomial theorem). *Let $x, y \in \mathbb{C}$ and $n \in \mathbb{N}$, then*

$$(x+y)^n = \sum_{k=0}^{n} \binom{n}{k} x^{n-k} y^k. \tag{A.4}$$

Result A.5 (Gamma and beta function). *For $x > 0$, the gamma function is defined by*

$$\Gamma(x) := \int_0^\infty t^{x-1} e^{-t} dt. \tag{A.5}$$

Two properties of this integral are

- $\Gamma(n) = (n-1)!, \quad n \in \mathbb{N},$
- $\Gamma\left(\frac{n}{2}\right) = 2^{-\frac{1}{2}n+\frac{1}{2}} \sqrt{\pi}(n-2)!!, \quad n \in \mathbb{N},$ *n odd.*

Here $n!! = n(n-2)\cdots 1$. A function closely related to the gamma function is the beta function, for which we have

$$B(x_1, x_2) := \int_0^1 t^{x_1-1}(1-t)^{x_2-1} dt = \frac{\Gamma(x_1)\Gamma(x_2)}{\Gamma(x_1+x_2)} \tag{A.6}$$

Definition A.6 (Group)**.** *A group is a set* G *with an operation* $G \times G \to G$*, which we shall denote here as* $(a, b) \mapsto a \circ b$*, such that the following three requirements are met.*

(G1) *(Associativity) For all* $a, b, c \in G$ *we have that* $a \circ (b \circ c) = (a \circ b) \circ c$*.*

(G2) *(Identity element) There is an* $e \in G$ *such that* $e \circ a = a \circ e = a$*, for all* $a \in G$*.*

(G3) *(Inverse element) For every* $a \in G$ *there exists an element* $a^* \in G$ *such that* $a \circ a^* = a^* \circ a = e$*.*

Definition A.7 (Action)**.** *Let* G *be a group, and let* X *be a set. We say that* G acts on X *if for every* $g \in G$ *and every* $x \in X$*, an element* $g \circ x \in X$ *is given such that:*

(W0) $e \circ x = x \ \ \forall x \in X$*,*

(W1) $(gh) \circ x = g \circ (h \circ x) \ \ \forall g, h \in G$ *and* $x \in X$*.*

Definition A.8 (Stabiliser)**.** *Let the group* G *act on the set* X *and let* $x \in X$*. If* $g \circ x = x$*, then we say that* x *is a fixed point of* g*. The stabiliser of* x *in* G*, notation* G_x*, is the subset*

$$G_x = \{g \in G : g \circ x = x\}.$$

B

Elementary calculations

Proposition B.1. *Fix $m \in \mathbb{Z}$. Then for $\ell \neq n$, we have*

$$\langle \tilde{Y}_\ell^m, \tilde{Y}_n^m \rangle = 0$$

Proof. Since we are showing equality to zero we can choose $C = 1$ in (3.17). Now note that the inner product in (2.11) is defined for Cartesian coordinates. However, since $\tilde{Y}_\ell^m, \tilde{Y}_n^m$ are defined in spherical coordinates, we transform the integral. The Jacobian of this transformation is $r^2 \sin\theta$, so with $r = 1$ we see

$$\begin{aligned}\langle \tilde{Y}_\ell^m, \tilde{Y}_n^m \rangle &= \frac{1}{\sigma(S^2)} \int_{S^2} \tilde{Y}_\ell^m, \overline{\tilde{Y}_n^m} d\sigma = \frac{1}{4\pi} \int_0^{2\pi} \int_0^\pi P_\ell^m(\cos\theta) e^{im\phi} P_n^m(\cos\theta) e^{-im\phi} \sin\theta \; d\theta d\phi \\ &= \frac{1}{4\pi} \int_0^{2\pi} \int_0^\pi P_\ell^m(\cos\theta) P_n^m(\cos\theta) \sin\theta \; d\theta d\phi = \frac{2\pi}{4\pi} \int_0^\pi P_\ell^m(\cos\theta) P_n^m(\cos\theta) \sin\theta \; d\theta.\end{aligned}$$

Now we make a change of variables back to Cartesian coordinates with $x = \cos\theta$ and so $dx = \sin\theta \; d\theta$, which yields

$$\frac{1}{2} \int_{-1}^1 P_\ell^m(x) P_n^m(x) \; dx$$

To show that this integral equals 0, we resort back to the associated Legendre equation (3.14), which we can rewrite using the chain rule:

$$\frac{d}{dx}\left((1-x^2)\frac{dy}{dx}\right) + \left(\ell(\ell+1) - \frac{m^2}{1-x^2}\right) y = 0.$$

Now we know that $\tilde{Y}_\ell^m, \tilde{Y}_n^m$ satisfy this equation, so we can substitute them in and get

$$\frac{d}{dx}\left((1-x^2)\frac{d}{dx} P_\ell^m(x)\right) + \left(\ell(\ell+1) - \frac{m^2}{1-x^2}\right) P_\ell^m(x) = 0, \tag{B.1}$$

$$\frac{d}{dx}\left((1-x^2)\frac{d}{dx} P_n^m(x)\right) + \left(n(n+1) - \frac{m^2}{1-x^2}\right) P_n^m(x) = 0. \tag{B.2}$$

Multiply (B.1) with $P_n^m(x)$ and (B.2) with $P_\ell^m(x)$, then subtracting yields

$$P_n^m(x)\frac{d}{dx}\left((1-x^2)\frac{d}{dx}P_\ell^m(x)\right) - P_\ell^m(x)\frac{d}{dx}\left((1-x^2)\frac{d}{dx}P_n^m(x)\right) + (\ell(\ell+1) - n(n+1)) P_n^m(x) P_\ell^m(x) = 0.$$

Using the chain rule for the first term we can write

$$\frac{d}{dx}\left((1-x^2)\left(P_n^m(x)\frac{d}{dx}P_\ell^m(x) - P_\ell^m(x)\frac{d}{dx}P_n^m(x)\right)\right) + (\ell(\ell+1) - n(n+1)) P_n^m(x) P_\ell^m(x) = 0.$$

Now integrating gives

$$\int_{-1}^{1} \frac{d}{dx}\left((1-x^2)\left(P_n^m(x)\frac{d}{dx}P_\ell^m(x) - P_\ell^m(x)\frac{d}{dx}P_n^m(x)\right)\right) dx + (\ell(\ell+1) - n(n+1))\int_{-1}^{1} P_n^m(x)P_\ell^m(x)\ dx$$
$$= \left[(1-x^2)\left(P_n^m(x)\frac{d}{dx}P_\ell^m(x) - P_\ell^m(x)\frac{d}{dx}P_n^m(x)\right)\right]_{-1}^{1} + (\ell(\ell+1) - n(n+1))\int_{-1}^{1} P_n^m(x)P_\ell^m(x)\ dx = 0.$$

Finally, note that $1 - x^2 = 0$ for $x = -1, 1$, so we get

$$(\ell(\ell+1) - n(n+1))\int_{-1}^{1} P_n^m(x)P_\ell^m(x)\ dx = 0.$$

Thus we can conclude that, for $\ell \neq n$, $\langle \tilde{Y}_\ell^m, \tilde{Y}_n^m \rangle = 0$. □